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The structure of graphs with given number of blocks and the maximum Wiener index

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Abstract

The Wiener index (the distance) of a connected graph is the sum of distances between all pairs of vertices. In this paper, we study the maximum possible value of this invariant among graphs on n vertices with fixed number of blocks p. It is known that among graphs on n vertices that have just one block, the n-cycle has the largest Wiener index. And the n-path, which has $n-1$ blocks, has the maximum Wiener index in the class of graphs on n vertices. We show that among all graphs on n vertices which have $p \geq 2$ blocks, the maximum Wiener index is attained by a graph composed of two cycles joined by a path (here we admit that one or both cycles can be replaced by a single edge, as in the case $p = n - 1$ for example).

Keywords Graph theory · Wiener index · Distance

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1 Introduction

Let G be a simple graph. By $V(G)$ and $E(G)$ we denote the vertex set and the edge set of G, respectively. Let u and v be two vertices of G. The length of a shortest $u-v$ path is denoted by $d_G(u,v)$, or simply by $d(u,v)$ if no confusion is likely, and is called the distance from u to v in G. The Wiener index is defined as the sum of the distances between all (unordered) pairs of vertices of G,

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v).$$

The *transmission* of a vertex v is the sum of the distances from v to other vertices of G, i.e., $w_G(v) = \sum_{u \in V(G)} d_G(u,v)$. Then the Wiener index of G equals $\frac{1}{2}\sum_{u \in G} w_G(u)$.

The Wiener index was introduced by Wiener (1947), thus it is one of the oldest topological descriptors. At first it was used for predicting the boiling points of paraffins, later some other applications of the Wiener index were revealed. Many years later it was studied also from a purely graph-theoretical point of view. But mathematicians studied the Wiener index under different names, such as the gross status (Harary 1959), the distance of a graph (Entringer et al. 1976) and the transmission (Šoltés 1991). More details can be found in some of the many surveys, see e.g. Dobrynin et al. (2001), Knor and Škrekovski (2014), Knor et al. (2016) and Xu et al. (2014).

Let G be a connected graph. A vertex v is a *cut-vertex* if we obtain a disconnected graph after removing v and its adjacent edges from G. G is *2-connected* if for every two vertices, say u and v, there is a cycle containing both u and v in G. A *block* is a maximal subgraph of G which does not have cut-vertices. Observe that a block is either an edge or a 2-connected subgraph of G. By *connected union of blocks* we mean a connected subgraph of G which is a union of several (at least one) blocks.

If G is a connected graph and v is a cut-vertex that partitions G into subgraphs G_1 and G_2, i.e., $G = G_1 \cup G_2$ and $G_1 \cap G_2 = \{v\}$, then we write $G = G_1 \circ_v G_2$, or simply $G = G_1 \circ G_2$. By C_n, P_n and K_n we denote a cycle, path and a complete graph, respectively, on n vertices. Our main result is the following statement.

Theorem 1.1 *Let n and p be numbers such that $n > p > 1$. Among all graphs on n vertices with p blocks, the maximum Wiener index is attained by the graph $H_a \circ_u P_{p-1} \circ_v H'_b$, where $|V(H_a)| = a$, $|V(H'_b)| = b$, $a, b \geq 2$, $a + b + p = n + 3$, H_a (H'_b) is a complete graph if $a = 2$ (if $b = 2$) or a cycle otherwise, and u and v are distinct endvertices of P_{p-1}.*

Hence, if $p = n - 1$ then the extremal graph is P_n, otherwise it is $C_a \circ_u P_p$ or $C_a \circ_u P_{p-1} \circ_v C_b$. The proof of Theorem 1.1 is rather technical. Therefore, the exact values of a and b will be determined in a forthcoming paper (Bessy et al. 2019). Let $W_n(p)$ be the maximum Wiener index of a graph which has n vertices and p blocks. In Bessy et al. (2019) we study $W_n(p)$ and we determine its minimum values.

Now, we introduce notations and definitions which we use throughout the paper. If $G, G_0, G_1, \ldots$ are graphs, we denote by $n, n_0, n_1, \ldots$, respectively, their numbers of vertices. For $v \in V(G)$, by $e_G(v)$ we denote the *eccentricity* of v in G, i.e., the maximal distance from v in G.

A graph is *non-separable* if it is connected and has no cut-vertices (i.e. either it is 2-connected or it is K_2). A *block* of G is a maximal non-separable subgraph of G. Two blocks sharing a common vertex are said to be *adjacent*. We refer to Bondy and Murty (2008) concerning the structure of blocks in a connected graph. In particular, it is known that the bipartite graph built on the set of blocks of G and the set of cut-vertices of G by linking a block to the cut-vertices it contains, is a tree. This tree is called the *blocks-tree* of G.

Let H be a subgraph of G, such that H is a connected union of several (at least one) blocks of G. An *attachment vertex* of H is a vertex of H which has a neighbour in $G \backslash H$. The subgraph H is *terminal* if H contains exactly one attachment vertex. It is *traversal* if it contains exactly two attachment vertices.

Let G be a connected graph on n vertices. The *distance vector* of a vertex v is the $e_G(v)$-dimensional vector $\boldsymbol{d}_G(v)$ given by $\boldsymbol{d}_G(v)_i = |\{x \in G : d_G(v, x) = i\}|$. If $\boldsymbol{v}$ is a vector with coordinates $\boldsymbol{v}_i$, then $\langle \boldsymbol{v} \rangle$ is the value $\sum_i i\boldsymbol{v}_i$. Observe that $\langle \boldsymbol{d}_G(v) \rangle = w_G(v)$.

Now we define $\mathbf{2}_n$. If n is even, the vector $\mathbf{2}_n$ has dimension $n/2$ and contains the value 2 in each coordinate except for the last one which is 1. If n is odd, $\mathbf{2}_n$ has dimension $(n-1)/2$ and each of its coordinates has value 2. For example $\mathbf{2}_7 = (2, 2, 2)$ and $\mathbf{2}_6 = (2, 2, 1)$. Observe that the vectors $\boldsymbol{d}_{C_n}(x)$ and $\mathbf{2}_n$ are the same for every vertex x of the cycle C_n. Hence we obtain $w_{C_n}(x) = \frac{n^2}{4}$ if n is even and $w_{C_n}(x) = \frac{n^2-1}{4}$ if n is odd. Also observe that if G is a 2-connected graph, then the distance vector of every vertex v of G satisfies $\boldsymbol{d}_G(v)_i \geq 2$ for every $i < e_G(v)$, and so $w_G(v) \leq \langle \mathbf{2}_n \rangle$. Moreover, if G is different from a cycle then it has a vertex u, such that $\boldsymbol{d}_G(u)_1 \geq 3$, which means that $w_G(u) < \langle \mathbf{2}_n \rangle$. So we get the following classical result.

Proposition 1.2 *Let G be a 2-connected graph on n vertices and let $v \in V(G)$. Then*

$$w_G(v) \leq \begin{cases} \frac{n^2}{4} & \text{if } n \text{ is even;} \\ \frac{n^2-1}{4} & \text{if } n \text{ is odd.} \end{cases}$$

Moreover, if G is C_n then equality holds for every vertex $v \in V(C_n)$. Further, the cycle C_n is the unique graph which has the maximal Wiener index over the class of 2-connected graphs on n vertices, and

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

We use also the following obvious statement.

Proposition 1.3 *Let v be an endvertex of P_n. Then*

$$w_{P_n}(v) = \binom{n}{2} \quad \text{and} \quad W(P_n) = \binom{n+1}{3}.$$

2 Proof of Theorem 1.1

In this section we prove Theorem 1.1 using a couple of auxiliary results. The first two propositions will be useful to calculate Wiener index of a graph composed of two or more subgraphs joined by cut-vertices. The proofs are straightforward, so we omit them. Recall that the number of vertices of G_i is denoted by n_i.

Proposition 2.1 *Let $G = G_1 \circ_v G_2$. We have*

$$W(G) = W(G_1) + W(G_2) + w_{G_1}(v) \cdot (n_2 - 1) + w_{G_2}(v) \cdot (n_1 - 1).$$

Observe that the subgraphs G_1 and G_2 in the previous proposition do not need to be blocks. In fact, each of these graphs is either a block or a connected union of blocks of G. Using an inductive argument we can get the following generalization of Proposition 2.1.

Proposition 2.2 *Let $G_1, G_2, \ldots, G_\ell$ be blocks or connected unions of blocks of G, such that $E(G_1), E(G_2), \ldots, E(G_\ell)$ is an edge decomposition of $E(G)$. Denote by $v_{i,j}$ the attachment vertex of G_i which separates G_i from G_j. Then*

$$\begin{aligned} W(G) = \sum_{i=1}^{\ell} W(G_i) + \sum_{1\le i<j\le \ell} \big(& w_{G_i}(v_{i,j}) \cdot (n_j - 1) \\ & + w_{G_j}(v_{j,i}) \cdot (n_i - 1) + d_G(v_{i,j}, v_{j,i}) \cdot (n_i - 1) \cdot (n_j - 1)\big). \end{aligned} \tag{1}$$

Observe that the last term in the second sum of Proposition 2.2 is 0 if G_i and G_j are adjacent blocks. We remark that Proposition 2.2 holds even in the case when some of the G_i are "trivial", i.e., if they consist of a single vertex, since then all the terms containing $W(G_i)$, $(n_i - 1)$, or $w_{G_i}(v_{i,j})$ are zeros.

Now we show that terminal blocks are cycles or edges in extremal graphs.

Lemma 2.3 *Let B be a terminal block of G such that B is not a cycle and $|V(B)| \geq 3$. Let G' be the graph obtained from G by replacing B by a cycle on $|V(B)|$ vertices. Then $W(G') > W(G)$.*

Proof Denote by v the attachment vertex of B in G. Further, denote by G_1 the block B and denote by G_2 the subgraph of G such that $G_1 \circ_v G_2 = G$. By Proposition 2.1 we have (recall that $n_i = |V(G_i)|$)

$$\begin{aligned} W(G) &= W(B) + W(G_2) + w_B(v) \cdot (n_2 - 1) + w_{G_2}(v) \cdot (n_1 - 1) \\ W(G') &= W(C_{n_1}) + W(G_2) + w_{C_{n_1}}(v) \cdot (n_2 - 1) + w_{G_2}(v) \cdot (n_1 - 1) \end{aligned}$$

and so

$$W(G') - W(G) = W(C_{n_1}) - W(B) + \big(w_{C_{n_1}}(v) - w_B(v)\big) \cdot (n_2 - 1).$$

Since B is not a cycle, we have $W(C_{n_1}) - W(B) > 0$ by Proposition 1.2. Moreover, by Proposition 1.2 we have also $w_{C_{n_1}}(v) = \langle \mathbf{2}_{n_1} \rangle \geq \langle \boldsymbol{d}_B(v) \rangle = w_B(v)$. Hence we obtain $W(G') > W(G)$. □

In a cycle C_n, two vertices u and v are *opposite* (or *antipodal*) if they satisfy $d_{C_n}(u, v) = \max\{d_{C_n}(x, y) : x, y \in C_n\} = \lfloor \frac{n}{2} \rfloor$. In K_2, two vertices are *opposite* if they are different.

Lemma 2.4 *Let B be a traversal block of G with $|V(B)| = n_0 \geq 3$, and let v_1 and v_2 be the two attachment vertices of B. Let C_{n_0} be a cycle in which v_1 and v_2 are opposite and let G' be obtained from G by replacing B by C_{n_0}. If B is not a cycle or if B is a cycle and v_1 and v_2 are not opposite in B, then $W(G') > W(G)$.*

Proof Denote by G_1 and G_2 the subgraphs of G attached to B at v_1 and v_2, respectively, such that $E(G) = E(G_1) \cup E(B) \cup E(G_2)$. By Proposition 2.2 we have

$$\begin{aligned} W(G') - W(G) = &\big(W(C_{n_0}) - W(B)\big) + \big(w_{C_{n_0}}(v_1) - w_B(v_1)\big) \cdot (n_1 - 1) \\ &+ \big(w_{C_{n_0}}(v_2) - w_B(v_2)\big) \cdot (n_2 - 1) \\ &+ \big(d_{C_{n_0}}(v_1, v_2) - d_B(v_1, v_2)\big) \cdot (n_1 - 1) \cdot (n_2 - 1). \end{aligned}$$

By Proposition 1.2 we have $W(C_{n_0}) - W(B) \geq 0$ and equality holds if and only if B is a cycle. By Proposition 1.2 we have also $w_{C_{n_0}}(v_1) - w_B(v_1) \geq 0$ and $w_{C_{n_0}}(v_2) - w_B(v_2) \geq 0$. Finally, since every vertex v in a 2-connected graph H satisfies $e_H(v) \leq \left\lfloor \frac{|V(H)|}{2} \right\rfloor$ (recall that for every $i < e_H(v)$ we have $\boldsymbol{d}_H(v)_i \geq 2$), we have $d_B(v_1, v_2) \leq \lfloor \frac{n_0}{2} \rfloor = d_{C_{n_0}}(v_1, v_2)$. Hence, all the terms on the right hand side of the equality for $W(G') - W(G)$ are nonnegative and they are all zeros if and only if $B = C_{n_0}$ and $d_B(v_1, v_2) = \lfloor \frac{n_0}{2} \rfloor$. □

By Lemma 2.3, a terminal block is either K_2 or a cycle. Next lemma gives a condition for extremal graphs.

Lemma 2.5 *Let G be a graph with at least 3 blocks and let G_1 and G_2 be two terminal blocks of G with attachment vertices v_1 and v_2, respectively. Let u_i be a vertex opposite to v_i in G_i for $i \in \{1, 2\}$. Denote by G' (resp. G'') a graph obtained from G by removing the block G_1 (resp. G_2) and attaching it to u_2 (resp. u_1). Suppose that $W(G) \geq W(G')$ and $W(G) \geq W(G'')$. Then $d_G(u_1, u_2) \geq \frac{n-1}{2}$.*

Proof Let G_0 be the graph obtained from G by removing the blocks G_1 and G_2, such that $E(G) = E(G_1) \cup E(G_0) \cup E(G_2)$. Observe that G_0 does not need to be a single block, but it is a connected union of blocks. Anyway, $G = G_1 \circ_{v_1} G_0 \circ_{v_2} G_2$, $G' = G_0 \circ_{v_2} G_2 \circ_{u_2} G_1$ and $G'' = G_2 \circ_{u_1} G_1 \circ_{v_1} G_0$. By Proposition 2.2 we have

$$\begin{aligned} W(G) - W(G') = &\big(w_{G_2}(v_2) - w_{G_2}(u_2)\big) \cdot (n_1 - 1) + \big(w_{G_0}(v_1) - w_{G_0}(v_2)\big) \cdot (n_1 - 1) \\ &+ d_{G_0}(v_1, v_2) \cdot (n_1 - 1) \cdot (n_2 - 1) - d_{G_2}(v_2, u_2) \cdot (n_1 - 1) \cdot (n_0 - 1) \end{aligned}$$

where $w_{G_2}(v_2) = w_{G_2}(u_2)$. Since $W(G) \geq W(G')$ and $n_1 \geq 2$, we get

$$w_{G_0}(v_1) - w_{G_0}(v_2) + d_{G_0}(v_1, v_2) \cdot (n_2 - 1) - d_{G_2}(v_2, u_2) \cdot (n_0 - 1) \geq 0.$$

Analogously, from $W(G) - W(G'') \geq 0$ we get

$$w_{G_0}(v_2) - w_{G_0}(v_1) + d_{G_0}(v_1, v_2) \cdot (n_1 - 1) - d_{G_1}(v_1, u_1) \cdot (n_0 - 1) \geq 0$$

and summing the last two inequalities we obtain

$$d_G(v_1, v_2) \cdot (n_1 + n_2 - 2) - \big(d_{G_2}(v_2, u_2) + d_{G_1}(v_1, u_1)\big) \cdot (n_0 - 1) \geq 0.$$

Now since v_i and u_i are opposite in G_i for $i \in \{1, 2\}$, we have

$$d_G(v_1, u_1) + d_G(v_2, u_2) = \left\lfloor \frac{n_1}{2} \right\rfloor + \left\lfloor \frac{n_2}{2} \right\rfloor \geq \frac{n_1 - 1}{2} + \frac{n_2 - 1}{2} = \frac{n_1 + n_2 - 2}{2}.$$

Thus we obtain $d_G(v_1, v_2) \geq (n_0 - 1)/2$ and consequently

$$\begin{aligned} d_G(u_1, u_2) &= d_G(u_1, v_1) + d_G(v_1, v_2) + d_G(v_2, u_2) \\ &\geq \frac{n_1 - 1}{2} + \frac{n_0 - 1}{2} + \frac{n_2 - 1}{2} = \frac{n - 1}{2} \end{aligned}$$

since $n = n_1 + n_0 + n_2 - 2$. □

Let $n = tk + 1$. Take k paths of length t (i.e. on $t + 1$ vertices), on each path choose one endvertex, and identify these endvertices. We denote by R_n^k the resulting graph. Observe that R_n^k has n vertices and is homeomorphic to the star $K_{1,k}$. In Knor and Škrekovski (2019, Theorem 3) we have the following statement.

Theorem 2.6 *Let G be a connected graph on n vertices. Then for every k-tuple $u_1, u_2, \ldots, u_k$ of its vertices, $3 \leq k < n$, there are two, say u_i and u_j where $1 \leq i < j \leq k$, such that*

$$d_G(u_i, u_j) \leq \frac{2n - 2}{k}.$$

Moreover, if

$$\min_{1 \leq i < j \leq k} d_G(u_i, u_j) = \frac{2n - 2}{k}$$

then $n \equiv 1 \pmod{k}$, the graph is R_n^k and $u_1, u_2, \ldots, u_k$ are the endvertices of R_n^k.

Using Theorem 2.6 and Lemma 2.5 we prove the following statement.

Lemma 2.7 *Let $n > p$. Let G be a graph on n vertices with p blocks which has the maximum Wiener index. Then G has at most three terminal blocks.*

Proof By way of contradiction, suppose that G has at least four terminal blocks, say B_1, B_2, B_3 and B_4. By Lemma 2.3 we know that each of these blocks is either a cycle or K_2. Let v_i be the unique attachment vertex of B_i and let u_i be a vertex opposite to v_i in B_i, $1 \leq i \leq 4$. Denote

$$d = \min_{1 \leq i < j \leq 4} d_G(u_i, u_j)$$

and assume that this minimum is attained by the pair u_1, u_2. By Theorem 2.6 we know that $d \leq \frac{n-1}{2}$. We distinguish two cases.

Case 1: $d < \frac{n-1}{2}$. Denote $G_1 = B_1$ and $G_2 = B_2$. Now construct G' and G'' by reattaching of G_1 and G_2 as in Lemma 2.5. Since $d_G(u_1, u_2) = d < \frac{n-1}{2}$, either $W(G) < W(G')$ or $W(G) < W(G'')$. Since all G, G' and G'' have n vertices and p blocks, we get a contradiction.

Case 2: $d = \frac{n-1}{2}$. By Theorem 2.6, in this case G is R_n^4, and so $p = n - 1$. It is well-known that among trees on n vertices, P_n is the unique graph with the maximum Wiener index. So $W(P_n) > W(R_n^4)$, a contradiction. □

Now we prove some results useful for sequences of traversal blocks. The following theorem was proved in Gutman et al. (2014).

Theorem 2.8 *For every $n \notin \{7, 9\}$, the graph $C_{n-2} \circ C_3$ has the maximal Wiener index among the graphs from the family $\{C_{n-r+1} \circ C_r : r \geq 3,\ n - r \geq 2\}$. Moreover for $n = 7$ and $n = 9$, it holds $W(C_4 \circ C_4) > W(C_5 \circ C_3)$ and $W(C_6 \circ C_4) > W(C_7 \circ C_3) > W(C_5 \circ C_5)$.*

We extend Lemma 2.8 to blocks of size 2.

Lemma 2.9 *For every $n \geq 4$, among the graphs on n vertices with exactly two blocks, the maximal Wiener index is attained by $C_{n-1} \circ K_2$.*

Proof For $n = 4$ the graph $C_3 \circ K_2$ is the unique graph with two blocks, thus it has the largest Wiener index. For $n \geq 5, n \notin \{7, 9\}$, it is enough to show that $W(C_{n-1} \circ K_2) > W(C_{n-2} \circ C_3)$, by Theorem 2.8.

Using Proposition 2.1 we get the Wiener index of $G = C_{n-1} \circ_v K_2$.

$$\begin{aligned} W(G) &= W(C_{n-1}) + W(K_2) + w_{C_{n-1}}(v) \cdot 1 + w_{K_2}(v) \cdot (n-2) \\ &= \tfrac{n-1}{2} \langle \mathbf{2}_{n-1} \rangle + 1 + \langle \mathbf{2}_{n-1} \rangle \cdot 1 + 1 \cdot (n-2). \end{aligned}$$

In $G' = C_{n-2} \circ_u C_3$ we can also use Proposition 2.1 to evaluate the Wiener index.

$$\begin{aligned} W(G') &= W(C_{n-2}) + W(C_3) + w_{C_{n-2}}(u) \cdot 2 + w_{C_3}(u) \cdot (n-3) \\ &= \tfrac{n-2}{2} \langle \mathbf{2}_{n-2} \rangle + 3 + \langle \mathbf{2}_{n-2} \rangle \cdot 2 + 2 \cdot (n-3). \end{aligned}$$

Hence, using Proposition 1.2 we get

$$W(G) - W(G') = \tfrac{n+1}{2} \langle \mathbf{2}_{n-1} \rangle - \tfrac{n+2}{2} \langle \mathbf{2}_{n-2} \rangle - n + 2$$

$$= \begin{cases} \frac{(n-2)(n-4)}{8} & \text{if } n \text{ is even;} \\ \frac{(n-1)(n-3)}{8} + 1 & \text{if } n \text{ is odd.} \end{cases}$$

Since $n \geq 5$, in both cases we get $W(G) > W(G')$.

By Theorem 2.8, for $n = 7$ and $n = 9$ it suffices to show that $W(C_{n-1} \circ K_2) > W(C_{n-3} \circ C_4)$. Direct computation gives $W(C_4 \circ C_4) = 40$, $W(C_6 \circ K_2) = 42$, $W(C_6 \circ C_4) = 82$ and $W(C_8 \circ K_2) = 88$, which completes the proof. □

Using Lemma 2.9 we prove the following statement. Here we allow the smaller end-block to be just a single vertex, i.e. $|V(G_0)| = 1$, see below. For technical reasons, we denote K_2 by C_2. Observe that if $u \in V(K_2)$ then $w_{K_2}(u) = 1 = \frac{|V(K_2)|^2}{4}$ and $W(K_2) = 1 = \frac{|V(K_2)|^3}{8}$. Hence, this notation is in a correspondence with Proposition 1.2.

Lemma 2.10 *Let $G = G_0 \circ_{v_1} G_1 \circ_v G_2 \circ_{v_2} G_3$, where G_1 and G_2 are C_{n_1} and C_{n_2}, respectively, v_1 and v are antipodal in G_1, and v and v_2 are antipodal in G_2. Let $k = n_1 + n_2 - 1$, $n_0 \leq n_3$ and $n_3 \geq 2$. Then G has maximal Wiener index if and only if*

1. *$n_1 = k - 1$ and $n_2 = 2$, or*
2. *$n_1 = 2$, $n_2 = k - 1$ and $n_0 = n_3$.*

Proof Let $G' = G_0 \circ_{v_1} C_{n_1+n_2-2} \circ_u C_2 \circ_{v_2} G_3$, where u is antipodal to v_1 in $C_{n_1+n_2-2}$ and u is antipodal to (i.e., different from) v_2 in C_2 $(= K_2)$. Denote $H = C_{n_1} \circ C_{n_2}$ and $H' = C_{n_1+n_2-2} \circ C_2$. By Proposition 2.2 we have

$$\begin{aligned} W(G') - W(G) = &\big(W(H') - W(H)\big) + \big(w_{H'}(v_1) - w_H(v_1)\big) \cdot (n_0 - 1) \\ &+ \big(w_{H'}(v_2) - w_H(v_2)\big) \cdot (n_3 - 1) \\ &+ \big(d_{H'}(v_1, v_2) - d_H(v_1, v_2)\big) \cdot (n_0 - 1) \cdot (n_3 - 1). \end{aligned}$$

By Lemma 2.9 we have $W(H') - W(H) \geq 0$ and equality holds if and only if $H = H'$ (i.e., if $n_1 = 2$ or if $n_2 = 2$). Further, $d_{H'}(v_1, v_2) = \lfloor \frac{n_1+n_2-2}{2} \rfloor + \lfloor \frac{2}{2} \rfloor \geq \lfloor \frac{n_1}{2} \rfloor + \lfloor \frac{n_2}{2} \rfloor = d_H(v_1, v_2)$, and so the last term is nonnegative as well. Let

$$\Delta = \big(w_{H'}(v_1) - w_H(v_1)\big) \cdot (n_0 - 1) + \big(w_{H'}(v_2) - w_H(v_2)\big) \cdot (n_3 - 1).$$

We show that $\Delta \geq 0$.

If k is even, we have $w_{H'}(v_1) = \langle \boldsymbol{d}_{H'}(v_1) \rangle = \langle (2, 2, \ldots, 2, 1) \rangle$, and $w_{H'}(v_2) = \langle \boldsymbol{d}_{H'}(v_2) \rangle = \langle (1, 2, 2, \ldots, 2) \rangle$, where these vectors both have dimension $k/2$. If k is odd, we get $w_{H'}(v_1) = \langle \boldsymbol{d}_{H'}(v_1) \rangle = \langle (2, 2, \ldots, 2, 1, 1) \rangle$, and $w_{H'}(v_2) = \langle \boldsymbol{d}_{H'}(v_2) \rangle = \langle (1, 2, 2, \ldots, 2, 1) \rangle$, where both these vectors have dimension $(k+1)/2$. To compute $w_H(v_1)$, $w_H(v_2)$ and Δ we distinguish four cases according to the parity of k and n_1.

Case 1: *Both k and n_1 are even.* Then n_2 is odd and $w_H(v_1) = \langle \boldsymbol{d}_H(v_1) \rangle = \langle (2, \ldots, 2, 1, 2, \ldots, 2) \rangle$, where $\boldsymbol{d}_H(v_1)$ is a vector of dimension $k/2$, such that the $\frac{n_1}{2}$-

th coordinate is 1, i.e., $\boldsymbol{d}_H(v_1)_{n_1/2} = 1$, and $w_H(v_2) = \langle \boldsymbol{d}_H(v_2)\rangle = \langle(2,\ldots,2,1)\rangle$, where $\boldsymbol{d}_H(v_2)$ is also a vector of dimension $k/2$. So

$$\Delta = \big(\tfrac{n_1}{2} - \tfrac{k}{2}\big)(n_0 - 1) + \big(-1 + \tfrac{k}{2}\big)(n_3 - 1) = \tfrac{n_1-k}{2}\cdot(n_0-1) + \tfrac{k-2}{2}\cdot(n_3-1).$$

This is nonnegative since $n_0 \le n_3$ and $k-2 \ge k-n_1$. Moreover, $\Delta = 0$ if and only if $n_0 = n_3$ and $n_1 = 2$.

Case 2: *k is even and n_1 is odd.* Then n_2 is even and $w_H(v_1) = \langle \boldsymbol{d}_H(v_1)\rangle = \langle(2,\ldots,2,1)\rangle$, where $\boldsymbol{d}_H(v_1)$ is a vector of dimension $k/2$, and $w_H(v_2) = \langle \boldsymbol{d}_H(v_2)\rangle = \langle(2,\ldots,2,1,2,\ldots,2)\rangle$, where $\boldsymbol{d}_H(v_2)$ is also a vector of dimension $k/2$, in which $\boldsymbol{d}_H(v_2)_{n_2/2} = 1$. So

$$\Delta = 0\cdot(n_0-1) + \big(-1+\tfrac{n_2}{2}\big)(n_3-1) = \tfrac{n_2-2}{2}\cdot(n_3-1).$$

This is nonnegative since $n_2 - 2 \ge 0$. Moreover, $\Delta = 0$ if and only if $n_2 = 2$, since $n_3 \ge 2$.

Case 3: *k is odd and n_1 is even.* Then n_2 is even and $w_H(v_1) = \langle \boldsymbol{d}_H(v_1)\rangle = \langle(2,\ldots,2,1,2,\ldots,2,1)\rangle$, where $\boldsymbol{d}_H(v_1)$ is a vector of dimension $(k+1)/2$, such that $\boldsymbol{d}_H(v_1)_{n_1/2} = 1$ and $w_H(v_2) = \langle \boldsymbol{d}_H(v_2)\rangle = \langle(2,\ldots,2,1,2,\ldots,2,1)\rangle$, where $\boldsymbol{d}_H(v_2)$ is also a vector of dimension $(k+1)/2$, in which $\boldsymbol{d}_H(v_2)_{n_2/2} = 1$. Since $k-1-n_1 = n_2-2$, we have

$$\Delta = \big(\tfrac{n_1}{2} - \tfrac{k-1}{2}\big)(n_0-1) + \big(-1+\tfrac{n_2}{2}\big)(n_3-1) = \tfrac{n_2-2}{2}\cdot(n_3-n_0).$$

This is nonnegative since $n_2 \ge 2$ and $n_3 \ge n_0$. Moreover $\Delta = 0$ if and only if $n_2 = 2$ or $n_3 = n_0$.

Case 4: *Both k and n_1 are odd.* Then n_2 is odd and $w_H(v_1) = \langle \boldsymbol{d}_H(v_1)\rangle = w_H(v_2) = \langle \boldsymbol{d}_H(v_2)\rangle = \langle(2,\ldots,2)\rangle$, where both these vectors are of dimension $(k-1)/2$. So

$$\Delta = \big(\tfrac{-(k-1)}{2} + \tfrac{k+1}{2}\big)(n_0-1) + \big(-1+\tfrac{k+1}{2}\big)(n_3-1) = (n_0-1) + \tfrac{k-1}{2}\cdot(n_3-1) > 0.$$

Now combining these cases with Lemma 2.9, which states that $W(H') \ge W(H)$ and the equality holds if and only if $H = H'$ (see Case 3), yields the result. □

In the following lemma we consider chains of traversal blocks.

Lemma 2.11 *Let $n > p$. Let G be a graph on n vertices with p blocks which has the maximum Wiener index. Moreover, suppose that $G = H_0 \circ_{v_1} H_1 \circ_{v_2} \cdots \circ_{v_{\ell-1}} H_{\ell-1} \circ_{v_\ell} H_\ell$, where $\ell \ge 2$, all $H_0,\ldots,H_{\ell-1}$ are blocks and H_ℓ is a connected union of blocks. Then $|V(H_1)| = \cdots = |V(H_{\ell-2})| = 2$. Moreover, if H_ℓ is a terminal block or if $|V(H_0 \circ \cdots \circ H_{\ell-2})| \le |V(H_\ell)|$, then $|V(H_{\ell-1})| = 2$ as well.*

Proof Since H_0 is a terminal block and $H_1,\ldots,H_{\ell-1}$ are traversal, each of these blocks is either a cycle or K_2, by Lemmas 2.3 and 2.4. Moreover, by Lemma 2.4 we know that the attachment vertices v_i and v_{i+1} are opposite on H_i, $1 \le i \le \ell-1$.

Suppose that among $H_1, \dots, H_{\ell-2}$ there is a cycle on at least 3 vertices, say H_i. By Lemma 2.10 both H_{i-1} and H_{i+1} must be isomorphic to K_2. Denote $t_1 = |V(H_0 \circ \cdots \circ H_{i-1})|$ and $t_2 = |V(H_{i+1} \circ \cdots \circ H_\ell)|$. We distinguish two cases.

Case 1: $t_1 \leq t_2$. Denote $G_0 = H_0 \circ \cdots \circ H_{i-2}$, $G_1 = H_{i-1}$, $G_2 = H_i$ and $G_3 = H_{i+1} \circ \cdots \circ H_\ell$. (Observe that if $i = 1$ then G_0 is trivial consisting of a single vertex.) Then $n_0 = t_1 - 1 < t_2 = n_3$. Hence, by Lemma 2.10 we have $n_2 = 2$, a contradiction.

Case 2: $t_1 > t_2$. Denote $G_0 = H_\ell \circ \cdots \circ H_{i+2}$, $G_1 = H_{i+1}$, $G_2 = H_i$ and $G_3 = H_{i-1} \circ \cdots \circ H_0$. Then $n_0 = t_2 - 1 < t_1 = n_3$. Hence, by Lemma 2.10 we have $n_2 = 2$, a contradiction.

Now we consider $H_{\ell-1}$. If $|V(H_0 \circ \cdots \circ H_{\ell-2})| \leq |V(H_\ell)|$, then denote $G_0 = H_0 \circ \cdots \circ H_{\ell-3}$, $G_1 = H_{\ell-2}$, $G_2 = H_{\ell-1}$ and $G_3 = H_\ell$. (Observe that if $\ell = 2$ then G_0 is trivial.) Since $n_0 < n_3$, by Lemma 2.10 we have $n_2 = 2$.

If H_ℓ is a terminal block and $\ell \geq 3$, then relabelling the blocks (reversing their order) we can prove that $|V(H_{\ell-1})| = 2$.

Finally, if H_ℓ is a terminal block, $\ell = 2$ and $|V(H_0)| > |V(H_2)|$, then let G_0 be trivial, $G_1 = H_2$, $G_2 = H_1$ and $G_3 = H_0$. Then $n_0 < n_3$, and so $n_2 = 2$ by Lemma 2.10. □

By $\Theta_{a,b,c}$ we denote a graph consisting of two vertices, which are connected by three internally vertex-disjoint paths of lengths a, b and c. Observe that $\Theta_{a,b,c}$ has $a+b+c-1$ vertices. In Knor and Škrekovski (2019, Lemma 5) we have the following statement.

Theorem 2.12 *Let G be a 2-connected graph on n vertices, having three vertices v_1, v_2 and v_3 such that*

$$D = \sum_{1 \leq i < j \leq 3} d_G(v_i, v_j)$$

is maximum possible. Then $D \leq n + 1$ and the equality is attained only if G is $\Theta_{a,b,c}$, where all a, b and c are even.

Observe that if n is even then $D < n + 1$ by Theorem 2.12. Using this statement we prove the following lemma.

Lemma 2.13 *Let $n > p$. Let G be a graph on n vertices with p blocks which has the maximum Wiener index. Then G has exactly two terminal blocks.*

Proof By Lemma 2.7, G has at most three terminal blocks. By way of contradiction, suppose that G has exactly three terminal blocks. Then its blocks-tree has one vertex of degree 3, three vertices of degree 1 corresponding to terminal blocks, and all the remaining vertices have degree 2. The vertex of degree 3 corresponds either to a block or to a cut-vertex. To simplify the reasoning, in the latter case we consider the cut-vertex as a trivial block.

Hence, G consists of a block G_0 with three vertices v_1, v_2 and v_3 in which there are attached connected unions of blocks G_1, G_2 and G_3, respectively (obviously, the

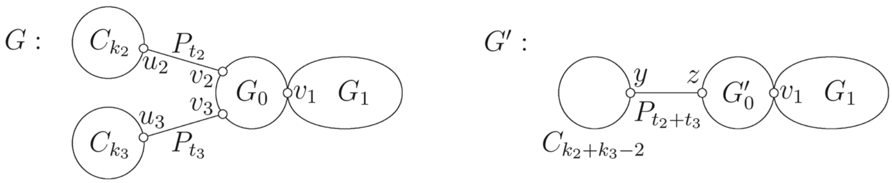

Fig. 1 Graphs G and G' in the proof of Lemma 2.13

vertices v_1, v_2 and v_3 are not necessarily disjoint). We assume that $n_1 \geq n_2 \geq n_3$. By Lemma 2.11, since $n_1 \geq n_i$ for $i \in \{2, 3\}$, we have $G_i = C_{k_i} \circ_{u_i} P_{t_i}$, where u_i is one endvertex of the path P_{t_i} and v_i is another one, and $k_i + t_i - 1 = n_i$. Observe that G_1 may consist of two cycles connected by a path, but we do not need to consider the structure of G_1. The structure of G is visualized on Fig. 1.

Now we construct G' on n vertices with p blocks, so that G' will have just two terminal blocks and $W(G') > W(G)$. First, if $n_0 \geq 3$, then let G'_0 be a cycle on n_0 vertices in which v_1 is opposite to z. If $n_0 \leq 2$, then G_0 is a cut vertex since the case $G_0 = K_2$ is impossible. So set $G'_0 = G_0$ and $z = v_1$ if $n_0 = 1$. Let z and y be the two endvertices of $P_{t_2+t_3}$. Then $G' = C_{k_2+k_3-2} \circ_y P_{t_2+t_3} \circ_z G'_0 \circ_{v_1} G_1$, see Fig. 1. Observe that the graphs G and G' have the same number of blocks and they have also the same number of vertices.

Since G' is simpler than G, we calculate $W(G')$ exactly. However, for $W(G)$ we use just an upper bound W. Below we show that $W(G') - W > 0$. Since $W(G) \leq W$, this implies that also $W(G') - W(G) > 0$.

By Proposition 1.3, $w_{P_a}(x) = \frac{a^2-a}{2}$ if x is an endvertex of a path of length a. But if x is a vertex of C_a then $w_{C_a}(x) = \frac{a^2}{4}$ if a is even and $W_{C_a}(x) = \frac{a^2-1}{4}$ if a is odd, see Proposition 1.2. Therefore, we distinguish two cases according to the parity of $k_2 + k_3 - 2$. If $k_2 + k_3 - 2$ is odd, then exactly one of k_2 and k_3 is odd as well. Since we do not use the inequality $n_2 \geq n_3$ in the proof, without loss of generality we may assume that k_2 is even and k_3 is odd in this case. If $k_2 + k_3 - 2$ is even, then either both k_2 and k_3 are even or both are odd. However, since it suffices to find an upper bound W on $W(G)$ such that $W(G') - W > 0$, we use the upper bounds $\frac{k_2^2}{4}$ and $\frac{k_3^2}{4}$ for $w_{C_{k_1}}(u_1)$ and $w_{C_{k_2}}(u_2)$, respectively, in this case.

Now we bound $W(G') - W(G)$ using Proposition 2.2. The graph G is composed of six parts C_{k_2}, P_{t_2}, C_{k_3}, P_{t_3}, G_0 and G_1, see Fig. 1. Therefore we have 6 terms in the first sum of (1), $2\binom{6}{2}$ terms due to the first two products in the second sum of (1) and $\binom{6}{2} - 5$ terms due to the third product in the second sum of (1). This yields 46 terms due to G. The graph G' is composed of four parts $C_{k_2+k_3-2}$, $P_{t_2+t_3}$, G'_0 and G_1, see Fig. 1. Therefore we have 19 terms due to G' in (1). Since there are too many terms, we divide them into several groups and we show that the sum of terms in each group is nonnegative.

1. First consider *the terms containing* $w_{G_1}(v_1)$. These terms occur in the first two products of the second sum of (1). In $W(G)$ these terms are $(k_2-1)w_{G_1}(v_1)$, $(t_2-1)w_{G_1}(v_1)$, $(k_3-1)w_{G_1}(v_1)$, $(t_3-1)w_{G_1}(v_1)$ and $(n_0-1)w_{G_1}(v_1)$. Observe that they sum to $(n-n_1)w_{G_1}(v_1)$. Since in $W(G')$ the three terms $(k_2+k_3-3)w_{G_1}(v_1)$,

$(t_2 + t_3 - 1)w_{G_1}(v_1)$ and $(n_0 - 1)w_{G_1}(v_1)$ containing $w_{G_1}(v_1)$ sum again to $(n - n_1)w_{G_1}(v_1)$, these terms contribute 0 to $W(G') - W(G)$.

2. Now consider *the terms containing* $w_{G_0}(v_1)$, $w_{G_0}(v_2)$, $w_{G_0}(v_3)$, $w_{G_0'}(v_1)$, *and* $w_{G_0'}(z)$. Since $w_{G_0'}(v_1) = w_{G_0'}(z)$, in $W(G')$ these terms sum to $(n - n_0)w_{G_0'}(v_1)$. By Proposition 1.2, we have $w_{G_0}(v_i) \le w_{G_0'}(v_1)$, $1 \le i \le 3$. Hence, the upper bound for the contribution of considered terms to $W(G)$ is also $(n - n_0)w_{G_0'}(v_1)$. Consequently, these terms contribute at least 0 to $W(G') - W(G)$.
3. Now consider *the terms containing* $(n_0 - 1)$ *which were not considered in the groups 1. and 2. above, together with the terms containing distances in* G_0 *and* G_0'. We start with the case when $k_2 + k_3 - 2$ is even.

First consider the terms containing $(n_0 - 1)$. Their contribution to $W(G') - W(G)$ is at least [the fractions correspond to $w_H(x)$'s, while the non-fractions correspond to the last term in (1)].

$$\begin{aligned}(n_0 - 1)\Big[&\tfrac{(k_2+k_3-2)^2}{4} + \tfrac{(t_2+t_3)^2-(t_2+t_3)}{2} + (k_2 + k_3 - 3)(t_2 + t_3 - 1)\\ &-\tfrac{k_2^2}{4} - \tfrac{k_3^2}{4} - \tfrac{t_2^2-t_2}{2} - \tfrac{t_3^2-t_3}{2} - (k_2 - 1)(t_2 - 1) - (k_3 - 1)(t_3 - 1)\Big]\\ = (n_0 - 1)&\Big[\tfrac{1}{2}(k_2 - 2)(k_3 - 2) + (k_2 - 2)t_3 + (k_3 - 2)t_2 + t_2t_3\Big]. \end{aligned} \tag{2}$$

Since $n_0 \ge 1$, $k_2 \ge 2$, $k_3 \ge 2$, $t_2 \ge 1$ and $t_3 \ge 1$, the expression (2) is nonnegative.

Now consider the terms containing distances in G_0 and G_0'. In $W(G)$ these terms sum to $(n_1 - 1)(n_2 - 1)d_{G_0}(v_1, v_2)$, $(n_1 - 1)(n_3 - 1)d_{G_0}(v_1, v_3)$ and $(n_2 - 1)(n_3 - 1)d_{G_0}(v_2, v_3)$. By Theorem 2.12 we have $d_{G_0}(v_1, v_2) + d_{G_0}(v_1, v_3) + d_{G_0}(v_2, v_3) \le n_0 + 1$. Since $n_1 \ge n_2$ and $n_1 \ge n_3$, we obtain the biggest contribution if $d_{G_0}(v_1, v_2)$ and $d_{G_0}(v_1, v_3)$ are maximum possible, namely $\lfloor \frac{n_0}{2} \rfloor$. Then $d_{G_0}(v_2, v_3) \le 2$. Hence, the contribution of these terms to $W(G)$ is at most

$$\Big\lfloor \frac{n_0}{2} \Big\rfloor \Big[(n_1 - 1)(n_2 - 1) + (n_1 - 1)(n_3 - 1)\Big] + 2(n_2 - 1)(n_3 - 1),$$

while the contribution of the terms containing $d_{G_0'}(v_1, z)$ to $W(G')$ is

$$d_{G_0'}(v_1, z)(n_1 - 1)(n_2 + n_3 - 2) = \Big\lfloor \frac{n_0}{2} \Big\rfloor (n_1 - 1)(n_2 + n_3 - 2).$$

Consequently, the contribution of these terms to $W(G') - W(G)$ is at least

$$-2(n_2 - 1)(n_3 - 1) = -2\Big[(k_2 - 2)(k_3 - 2) + (k_2 - 2)t_3 + (k_3 - 2)t_2 + t_2t_3\Big]. \tag{3}$$

Our aim is to show that the sum of the right-hand sides of (2) and (3) is nonnegative. We consider five cases.

Case 1: $n_0 \ge 5$. Since the expression in brackets containing k_2, k_3, t_2 and t_3 in (2) is nonnegative, it suffices to show nonnegativity of the sum of (2) and (3) for $n_0 = 5$. Since this sum is

$$2(k_2 - 2)t_3 + 2(k_3 - 2)t_2 + 2t_2t_3 > 0,$$

the contribution of selected terms is nonnegative in this case.

Case 2: $n_0 = 1$. In this case the considered distances in G_0 and G_0' are 0 as well as $(n_0 - 1)$. Hence, the contribution of selected terms is 0 in this case.

Case 3: $n_0 = 2$. This case is impossible, since if $G_0 = K_2$ then the vertex of degree 3 in the blocks-tree is a cut-vertex.

Case 4: $n_0 = 3$. In this case we have $d_{G_0}(v_i, v_j) = 1$, $1 \le i < j \le 3$, and also $d_{G_0'}(v_1, z) = 1$. Hence, the contribution of the terms based on distances is

$$-1\big[(k_2-2)(k_3-2) + (k_2-2)t_3 + (k_3-2)t_2 + t_2t_3\big]$$

and the total contribution of considered terms is

$$(k_2-2)t_3 + (k_3-2)t_2 + t_2t_3 > 0.$$

Case 5: $n_0 = 4$. By Theorem 2.12 we have $d_{G_0}(v_1, v_2)+d_{G_0}(v_1, v_3)+d_{G_0}(v_2, v_3) \le n_0 = 4$. In this case, the sum of the terms containing distances in G_0 and G_0' is non-negative. So the considered terms contribute to $W(G') - W(G)$ by at least

$$(n_0-1)\big[\tfrac{1}{2}(k_2-2)(k_3-2) + (k_2-2)t_3 + (k_3-2)t_2 + t_2t_3\big] > 0.$$

Summing up, the contribution of considered terms to $W(G') - W(G)$ is at least 0 if $k_2 + k_3 - 2$ is even. If $k_2 + k_3 - 2$ is odd, the only changes consist in replacing $\frac{(k_2+k_3-2)^2}{4}$ and $\frac{k_2^2}{4}$ by $\frac{(k_2+k_3-2)^2-1}{4}$ and $\frac{k_2^2-1}{4}$, respectively. Hence, we obtain exactly the same expressions as in the even case.

4. Now we consider *the terms containing* (n_1-1), *which were not considered before*. Again, we start with the case when $k_2 + k_3 - 2$ is even. The contribution of the terms containing $(n_1 - 1)$ is at least [compare with (2)]

$$\begin{aligned}(n_1-1)\Big[&\tfrac{(k_2+k_3-2)^2}{4} + \tfrac{(t_2+t_3)^2-(t_2+t_3)}{2} + (k_2+k_3-3)(t_2+t_3-1)\\ &-\tfrac{k_2^2}{4} - \tfrac{k_3^2}{4} - \tfrac{t_2^2-t_2}{2} - \tfrac{t_3^2-t_3}{2} - (k_2-1)(t_2-1) - (k_3-1)(t_3-1)\Big]\\ &= (n_1-1)\big[\tfrac{1}{2}(k_2-2)(k_3-2) + (k_2-2)t_3 + (k_3-2)t_2 + t_2t_3\big].\end{aligned}$$

Since the expression in brackets containing k_2, k_3, t_2 and t_3 is nonnegative, we can replace $(n_1 - 1)$ by a value which is not larger than $(n_1 - 1)$ and we will not increase the contribution of considered terms. Since $(n_1 - 1) \ge (n_i - 1) = (k_i + t_i - 2)$, $2 \le i \le 3$, we get $(n_1 - 1) \ge \frac{1}{2}(k_2 + k_3 + t_2 + t_3 - 4)$. Hence, the contribution of considered terms is at least

$$\tfrac{1}{2}(k_2+k_3+t_2+t_3-4)\big[\tfrac{1}{2}(k_2-2)(k_3-2) + (k_2-2)t_3 + (k_3-2)t_2 + t_2t_3\big] \tag{4}$$

if $k_2 + k_3 - 2$ is even. If $k_2 + k_3 - 2$ is odd, we obtain the very same expression.

5. Finally, we consider *the remaining terms, i.e., the terms which were not considered in the groups 1.–4. above*. Then we include the terms from (4) and we show that their sum is positive. Again, we start with the case when $k_2 + k_3 - 2$ is even.

Since $W(G_0') - W(G_0) \geq 0$, the terms from the first sum of Proposition 2.2 contribute to $W(G') - W(G)$ by at least

$$\frac{(k_2+k_3-2)^3}{8} + \frac{(t_2+t_3)^3-(t_2+t_3)}{6} - \frac{k_2^3}{8} - \frac{k_3^3}{8} - \frac{t_2^3-t_2}{6} - \frac{t_3^3-t_3}{6}. \tag{5}$$

The terms from the second sum of (1) contribute to $W(G') - W(G)$ by at least

$$\begin{aligned}
&\frac{(k_2+k_3-2)^2}{4}(t_2+t_3-1) + \frac{(t_2+t_3)^2-(t_2+t_3)}{2}(k_2+k_3-3)\\
&-\frac{k_2^2}{4}(k_3+t_2+t_3-3) - \frac{k_3^2}{4}(k_2+t_2+t_3-3) - \frac{t_2^2-t_2}{2}(k_2+k_3+t_3-3)\\
&-\frac{t_3^2-t_3}{2}(k_2+k_3+t_2-3) - (k_2-1)(k_3-1)(t_2+t_3-2)\\
&-(k_2-1)(t_3-1)(t_2-1) - (k_3-1)(t_2-1)(t_3-1).
\end{aligned} \tag{6}$$

And summing (4), (5) and (6) we get

$$\begin{aligned}
&\left(\frac{k_3-2}{4} + \frac{t_3-1}{2} + \frac{1}{2}\right)(k_2-2)^2 + \left(\frac{k_2-2}{4} + \frac{t_2-1}{2} + \frac{1}{2}\right)(k_3-2)^2\\
&+\left(\frac{k_3-2}{4} + \frac{t_3-1}{2}\right)(t_2-1)^2 + \left(\frac{k_2-2}{4} + \frac{t_2-1}{2}\right)(t_3-1)^2\\
&+\left(\frac{k_3^2-4}{8} + \frac{k_3t_3}{4} + t_2t_3\right)(k_2-2) + \left(\frac{k_2^2-4}{8} + \frac{k_2t_2}{4} + t_2t_3\right)(k_3-2)\\
&+\left(t_2^2-1\right)\frac{k_3}{4} + \left(t_3^2-1\right)\frac{k_2}{4} + 2(t_2-1)(t_3-1) + \frac{t_2}{2} + \frac{t_3}{2}
\end{aligned} \tag{7}$$

which is positive since all the terms are nonnegative while the last two are at least $\frac{1}{2}$ each.

Now consider the case when $k_2 + k_3 - 2$ is odd. Then (4) is without a change, (5) is increased by $-\frac{k_2+k_3-2}{8} + \frac{k_3}{8} = \frac{2-k_2}{8}$ and (6) is increased by $-\frac{1}{4}(t_2+t_3-1) + \frac{1}{4}(k_2+t_2+t_3-3) = \frac{k_2-2}{4}$. So the sum of considered terms is exactly as in (7) plus a nonnegative term $\frac{k_2-2}{8}$.

Since all the groups of terms are nonnegative and the last one is positive, the lemma is proved. □

Now combining Lemmas 2.11 and 2.13 we obtain Theorem 1.1.

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