Wiener index of iterated line graphs of trees homeomorphic to the claw $K_{1,3}$

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Abstract

Let G be a graph. Denote by $L^i(G)$ its i-iterated line graph and denote by $W(G)$ its Wiener index. Dobrynin, Entringer and Gutman stated the following problem: Does there exist a non-trivial tree T and $i \geq 3$ such that $W(L^i(T)) = W(T)$? In a series of five papers we solve this problem. In a previous paper we proved that $W(L^i(T)) > W(T)$ for every tree T that is not homeomorphic to a path, claw $K_{1,3}$ and to the graph of "letter H", where $i \geq 3$. Here we prove that $W(L^i(T)) > W(T)$ for every tree T homeomorphic to the claw, $T \neq K_{1,3}$ and $i \geq 4$.

1 Introduction

Let G be a graph. For any two of its vertices, say u and v, denote by $d_G(u,v)$ (or by $d(u,v)$ if no confusion is likely) the distance from u to v in G. The *Wiener index* of G, $W(G)$, is defined as

$$W(G) = \sum_{u \neq v} d(u,v),$$

where the sum is taken through all unordered pairs of vertices of G. Wiener index was introduced by Wiener in [12]. It is related to boiling point, heat of evaporation, heat of formation, chromatographic retention times, surface tension, vapour pressure, partition coefficients, total electron energy of polymers, ultrasonic sound

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velocity, internal energy, etc., see [8]. For this reason Wiener index is widely studied by chemists. The interest of mathematicians was attracted in 1970's. It was reintroduced as the distance and transmission, see [5] and [11], respectively. Recently, there are whole special issues of journals devoted to (mathematical properties) of Wiener index, see [6] and [7], as well as several surveys, see e.g. [3] and [4].

By definition, if G has a unique vertex, then $W(G) = 0$. In this case, we say that the graph G is *trivial*. We set $W(G) = 0$ also when the set of vertices (and hence also the set of edges) of G is empty.

The line graph of G, $L(G)$, has vertex set identical with the set of edges of G. Two vertices of $L(G)$ are adjacent if and only if the corresponding edges are adjacent in G. Iterated line graphs are defined inductively as follows:

$$L^i(G) = \begin{cases} G & \text{if } i = 0, \\ L(L^{i-1}(G)) & \text{if } i > 0. \end{cases}$$

In [1] we have the following statement.

Theorem 1.1 *Let T be a tree on n vertices. Then $W(L(T)) = W(T) - \binom{n}{2}$.*

Since $\binom{n}{2} > 0$ if $n \geq 2$, there is no nontrivial tree for which $W(L(T)) = W(T)$. However, there are trees T satisfying $W(L^2(T)) = W(T)$, see e.g. [2]. In [3], the following problem was posed:

Problem 1.2 *Is there any tree T satisfying the equality $W(L^i(T)) = W(T)$ for some $i \geq 3$?*

As observed above, if T is a trivial tree then $W(L^i(T)) = W(T)$ for every $i \geq 1$, although here the graph $L^i(T)$ is empty.

Denote by H the tree on six vertices out of which two have degree 3 and four have degree 1. Since H can be drawn to resemble the letter H, it is often called the H-graph. Graphs G_1 and G_2 are homeomorphic if and only if the graphs obtained from G_1 and G_2, respectively, by substituting the vertices of degree two together with the two incident edges with a single edge, are isomorphic. In [10] we proved the following:

Theorem 1.3 *Let T be a tree, not homeomorphic to a path, claw $K_{1,3}$ and the graph H. Then $W(L^i(T)) > W(T)$ for all $i \geq 3$.*

Since the case when T is a path is trivial, it remains to consider graphs homeomorphic to the claw $K_{1,3}$ and those homeomorphic to H. In this paper we concentrate on graphs homeomorphic to the claw $K_{1,3}$. The remaining two cases, namely the trees homeomorphic to H for $i \geq 3$ and trees homeomorphic to $K_{1,3}$ for $i = 3$, are dealt with in a forthcoming paper.

First, consider the case of the claw $K_{1,3}$ itself. Then $L^i(K_{1,3})$ is a cycle of length 3 for every $i \geq 1$. Since $W(K_{1,3}) = 9$ and the Wiener index of the cycle of length 3 is 3, we have $W(L^i(K_{1,3})) < W(K_{1,3})$ for every $i \geq 1$. For other trees homeomorphic to $K_{1,3}$, we prove the opposite inequality, provided that $i \geq 4$:

Theorem 1.4 *Let T be a tree homeomorphic to $K_{1,3}$, such that $T \neq K_{1,3}$. Then $W(L^i(T)) > W(T)$ for every $i \geq 4$.*

In [9] we proved the following statement:

Theorem 1.5 *Let G be a connected graph. Then $f_G(i) = W(L^i(G))$ is a convex function in variable i.*

Hence, to prove Theorem 1.4 it suffices to prove:

Theorem 1.6 *Let T be a tree homeomorphic to $K_{1,3}$, such that $T \neq K_{1,3}$. Then $W(L^4(T)) > W(T)$.*

2 Proofs

Let $a, b, c \geq 1$. Denote by $C_{a,b,c}$ a tree that has three paths of lengths a, b and c, starting at a common vertex of degree 3. Obviously, $C_{a,b,c}$ is homeomorphic to $K_{1,3}$ and $C_{1,1,1} = K_{1,3}$. By symmetry, we may assume $a \geq b \geq c$, see Figure 1 for $C_{5,4,3}$.

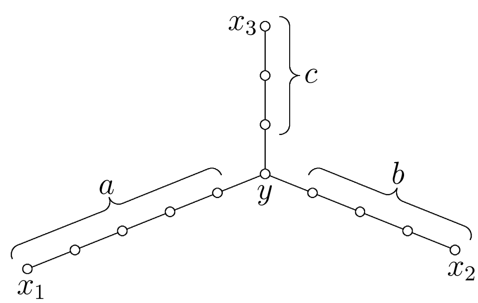

Figure 1: The graph $C_{5,4,3}$.

Denote

$$\Delta C_{a,b,c} = W(L^4(C_{a,b,c})) - W(C_{a,b,c}).$$

Our aim is to prove $\Delta C_{a,b,c} > 0$ if $a \geq 2$. We start with the case $a \leq 3$. This case will serve as the base of induction in the proof of Theorem 1.6.

Lemma 2.1 *Let $3 \geq a \geq b \geq c \geq 1$ and $a \neq 1$. Then $\Delta C_{a,b,c} > 0$.*

PROOF. Since $3 \geq a \geq b \geq c \geq 1$ and $a \neq 1$, there are 9 cases to consider. In Table 1 we present $\Delta C_{a,b,c}$ for each of these cases. The results were found by a computer, though it is rather easy to find $W(C_{a,b,c})$ by hand, and $W(L^4(C_{a,b,c}))$ can be found by applying Proposition 2.3 to $L^2(C_{a,b,c})$. $\square$

(a,b,c)	$W(C_{a,b,c})$	$W(L^4(C_{a,b,c}))$	$\Delta C_{a,b,c}$
$(3,3,3)$	138	642	504
$(3,3,2)$	102	533	431
$(3,3,1)$	75	257	182
$(3,2,2)$	72	435	363
$(3,2,1)$	50	192	142
$(3,1,1)$	32	65	33
$(2,2,2)$	48	348	300
$(2,2,1)$	31	138	107
$(2,1,1)$	18	38	20

Table 1: $\Delta C_{a,b,c}$ for $a \leq 3$.

In what follows we assume that $a \geq 4$. Denote

$$\begin{aligned}
\delta_0(a,b,c) &= W(C_{a,b,c}) - W(C_{a-1,b,c}) \\
\delta_4(a,b,c) &= W(L^4(C_{a,b,c})) - W(L^4(C_{a-1,b,c})).
\end{aligned}$$

Then

$$\Delta C_{a,b,c} - \Delta C_{a-1,b,c} = \delta_4(a,b,c) - \delta_0(a,b,c), \tag{1}$$

so if we prove $\delta_4(a,b,c) - \delta_0(a,b,c) \geq 0$, we obtain $\Delta C_{a,b,c} \geq \Delta C_{a-1,b,c}$.

We distinguish 4 vertices in $C_{a,b,c}$. Denote by y the vertex of degree 3, and denote by x_1, x_2 and x_3 the pendant vertices so that $d(x_1,y) = a$, $d(x_2,y) = b$ and $d(x_3,y) = c$, see Figure 1. As is the custom, by $V(G)$ we denote the vertex set of G.

Lemma 2.2 *Let $a,b,c \geq 1$. Then*

$$\delta_0(a,b,c) = \binom{a+b+1}{2} + \binom{a+c+1}{2} - \binom{a+1}{2}.$$

PROOF. Since $C_{a-1,b,c}$ is a subgraph of $C_{a,b,c}$ with $V(C_{a,b,c}) - V(C_{a-1,b,c}) = \{x_1\}$, we have

$$\delta_0(a,b,c) = W(C_{a,b,c}) - W(C_{a-1,b,c}) = \sum_u d(u,x_1),$$

where the sum goes through all $u \in V(C_{a,b,c}) \backslash \{x_1\}$. For vertices u of the $x_1 - x_2$ path, the sum of all $d(u,x_1)$ is $1+2+\cdots+(a+b) = \binom{a+b+1}{2}$. For vertices of the $x_1 - x_3$ path which do not lay on x_1-x_2 path, the sum of $d(u,x_1)$ is $(a+1)+(a+2)+\cdots+(a+c)=\binom{a+c+1}{2}-\binom{a+1}{2}$, see Figure 1. Since the paths x_1-x_2 and x_1-x_3 contain all vertices of $C_{a,b,c}$, we have $\delta_0(a,b,c)=\binom{a+b+1}{2}+\binom{a+c+1}{2}-\binom{a+1}{2}$. $\square$

For two subgraphs S_1 and S_2 of G, by $d(S_1,S_2)$ we denote the shortest distance in G between a vertex of S_1 and a vertex of S_2. If S_1 and S_2 share an edge then we set $d(S_1,S_2)=-1$.

Analogously as a vertex of $L(G)$ corresponds to an edge of G, a vertex of $L^2(G)$ corresponds to a path of length two in G. For $x\in V(L^2(G))$ we denote by $B_2(x)$ the corresponding path in G. Let x and y be two distinct vertices of $L^2(G)$. It was proved in [9] that

$$d_{L^2(G)}(x,y)=d_G(B_2(x),B_2(y))+2.$$

Let $u,v\in V(G)$, $u\neq v$. Denote by $\beta_i(u,v)$ the number of pairs $x,y\in V(L^2(G))$, with u being the center of $B_2(x)$ and v being the center of $B_2(y)$, such that $d(B_2(x),B_2(y))=d(u,v)-2+i$. Since $d(u,v)-2\le d(B_2(x),B_2(y))\le d(u,v)$, we have $\beta_i(u,v)=0$ for all $i\notin\{0,1,2\}$. Denote by $\deg(w)$ the degree of w in G. In [9] we have the following statement:

Proposition 2.3 *Let G be a connected graph. Then*

$$\begin{aligned} W(L^2(G)) &= \sum_{u\neq v}\left[\binom{\deg(u)}{2}\binom{\deg(v)}{2}d(u,v)+\beta_1(u,v)+2\beta_2(u,v)\right] \\ &+ \sum_{u}\left[3\binom{\deg(u)}{3}+6\binom{\deg(u)}{4}\right], \end{aligned} \tag{2}$$

where the first sum goes through unordered pairs $u,v\in V(G)$ and the second one goes through $u\in V(G)$.

We apply Proposition 2.3 to $L^2(C_{a,b,c})$ and $L^2(C_{a-1,b,c})$. This enables us to calculate $\delta_4(a,b,c)$ using degrees and distances of the second iterated line graph.

Denote by w_1 the pendant vertex of $L^2(C_{a,b,c})$ corresponding to the path of length 2 terminating at x_1. Since $a\ge 4$, the unique neighbour of w_1 has degree 2. Denote by w this neighbour, see Figure 2. For every vertex $u\in V(L^2(C_{a,b,c}))\setminus\{w,w_1\}$, denote by $n(u)$ the number of neighbours of u, whose distance to w is at least $d(u,w)$. We have:

Lemma 2.4 *Let $a\ge 4$ and $b,c\ge 1$. Then*

$$\delta_4(a,b,c)=\sum_u\left[\binom{\deg(u)}{2}d(u,w)+\binom{n(u)}{2}\right],$$

where the sum goes through all vertices of $V(L^2(C_{a,b,c}))\setminus\{w,w_1\}$.

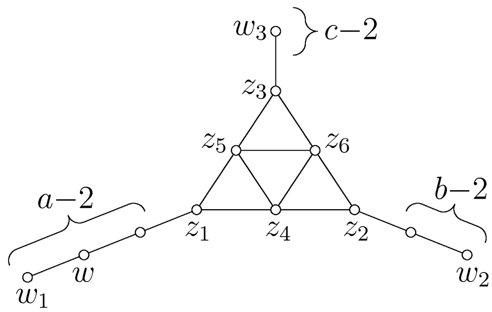

Figure 2: The graph $L^2(C_{5,4,3})$.

Proof. Observe that $L^2(C_{a-1,b,c})$ is a subgraph of $L^2(C_{a,b,c})$ and $V(L^2(C_{a,b,c}))\setminus V(L^2(C_{a-1,b,c}))=\{w_1\}$. Since $\deg(w_1)=1$, the vertex w_1 cannot be the center of a path of length 2, implying that $\beta_i(u,w_1)=0$ for every u and i. Since $\binom{\deg(w_1)}{2}=0$, all summands of (2) containing w_1 contribute 0 to $W(L^4(C_{a,b,c}))$. The vertices of $L^2(C_{a-1,b,c})$, except w, have the same degree in $L^2(C_{a,b,c})$ as in $L^2(C_{a-1,b,c})$. The degree of w is 1 in $L^2(C_{a-1,b,c})$, and it is 2 in $L^2(C_{a,b,c})$. Therefore $\sum_u[3\binom{\deg(u)}{3}+6\binom{\deg(u)}{4}]$ has the same value in $L^2(C_{a,b,c})$ as in $L^2(C_{a-1,b,c})$, so these sums will cancel out. Thus, we have

$$\begin{aligned}\delta_4(a,b,c) &= W(L^2(L^2(C_{a,b,c})))-W(L^2(L^2(C_{a-1,b,c})))\\ &= \sum_u\left[\binom{\deg(u)}{2}\binom{2}{2}d(u,w)+\beta_1(u,w)+2\beta_2(u,w)\right],\end{aligned}$$

where the sum goes through $u\in V(L^2(C_{a-1,b,c}))\setminus\{w\}$.

Let $u\in V(L^2(C_{a-1,b,c}))\setminus\{w\}$. Since $\deg(w_1)=1$ and $\deg(w)=2$ in $L^2(C_{a,b,c})$, the unique path of length 2 centered at w contains an endvertex closer to u than w. Hence, $\beta_2(u,w)=0$. Consequently, $\beta_1(u,w)$ equals the number of paths of length 2 centered at u, both endvertices of which have distance to w at least $d(u,w)$. Hence, $\beta_1(u,w)=\binom{n(u)}{2}$, which completes the proof. □

Using Lemma 2.4 we prove the induction step.

Lemma 2.5 *Let $a\ge b\ge c\ge 1$ and $a\ge 4$. Then $\delta_4(a,b,c)\ge\delta_0(a,b,c)$.*

Proof. We distinguish 8 more vertices in $L^2(C_{a,b,c})$. Denote by w_2 and w_3 pendant vertices corresponding to the paths of length 2 containing x_2 and x_3, respectively, see Figure 1 and 2. Denote by z_1, z_2 and z_3 the vertices corresponding to the paths of length 2, whose endvertex is y; and denote by z_4, z_5 and z_6 the vertices corresponding to the paths of length 2 centered at y. Of course, if $b \le 2$ or $c \le 2$, then some of these vertices are not defined.

For $u \in V(L^2(C_{a-1,b,c})) \setminus \{w\}$, denote

$$h(u) = \binom{\deg(u)}{2} d(u,w) + \binom{n(u)}{2}.$$

By Lemma 2.4, we have $\delta_4(a,b,c) = \sum_u h(u)$, where the sum goes through all vertices of $V(L^2(C_{a,b,c})) \setminus \{w, w_1\}$. If $u \in \{w_2, w_3\}$ then $\deg(u) = 1$ and $n(u) = 0$, so $h(u) = 0$. Thus, vertices of degree 1 contribute 0 to $\sum_u h(u)$. Denote

$$S_i = \sum_u h(u),$$

where the sum is taken over all interior vertices u of the $w_i - z_i$ path, $u \ne w$ and $1 \le i \le 3$. Then $\delta_4(a,b,c) = \sum_{i=1}^{3} S_i + \sum_{i=1}^{6} h(z_i)$.

Regarding the values of a, b and c, we distinguish 4 cases:

Case 1. *$a \ge 4$ and $b, c \ge 3$.*

If u is a vertex of degree 2, then $n(u) = 1$ and $\binom{\deg(u)}{2} = 1$. Hence $h(u) = d(u,w)$. Thus,

$$\begin{aligned} S_1 &= 1 + 2 + \cdots + (a-4) = \binom{a-3}{2} \\ S_2 &= a + (a+1) + \cdots + (a+b-4) = \binom{a+b-3}{2} - \binom{a}{2} \\ S_3 &= a + (a+1) + \cdots + (a+c-4) = \binom{a+c-3}{2} - \binom{a}{2}. \end{aligned}$$

If $u \in \{z_1, z_2, z_3\}$, then $\deg(u) = 3$ and $n(u) = 2$. Thus $h(u) = 3d(u,w) + 1$. If $u \in \{z_4, z_5\}$, then $\deg(u) = 4$ and $n(u) = 3$, so $h(u) = 6d(u,w) + 3$. Finally, if $u = z_6$, then $\deg(u) = 4$ and $n(u) = 2$, so $h(u) = 6d(u,w) + 1$. This gives

$$\begin{aligned} &h(z_1) = 3(a-3) + 1 && h(z_4) = h(z_5) = 6(a-2) + 3 \\ &h(z_2) = h(z_3) = 3(a-1) + 1 && h(z_6) = 6(a-1) + 1. \end{aligned}$$

Since $\delta_4(a,b,c) = \sum_{i=1}^{3} S_i + \sum_{i=1}^{6} h(z_i)$, we have

$$\begin{aligned} \delta_4(a,b,c) &= \binom{a-3}{2} + \binom{a+b-3}{2} + \binom{a+c-3}{2} - 2\binom{a}{2} \\ &\quad +(3a-8) + 2(3a-2) + 2(6a-9) + (6a-5). \end{aligned}$$

Denote $P = \delta_4(a,b,c) - \delta_0(a,b,c)$. By Lemma 2.2 we have $\delta_0(a,b,c) = \binom{a+b+1}{2} + \binom{a+c+1}{2} - \binom{a+1}{2}$. Expanding the terms we get

$$P = 17a - 4b - 4c - 17.$$

Since $a \ge b$ and $a \ge c$, we have $P \ge 9a - 17$. Finally, since $a \ge 4$, we have $P = \delta_4(a,b,c) - \delta_0(a,b,c) \ge 0$.

Case 2. *$a \geq 4$, $b \geq 3$ and $c \leq 2$.*

We calculate first $\delta_4(a,b,1)$. In $L^2(C_{a,b,1})$ we have $S_3 = 0$; note that z_3 is not defined here and that $\deg(z_5) = \deg(z_6) = 3$ (see Figure 2). Analogously as in Case 1 we get:

$$\begin{array}{ll}
S_1 = \binom{a-3}{2} & h(z_2) = 3(a-1)+1 \\
S_2 = \binom{a+b-3}{2} - \binom{a}{2} & h(z_4) = 6(a-2)+3 \\
S_3 = 0 & h(z_5) = 3(a-2)+1 \\
h(z_1) = 3(a-3)+1 & h(z_6) = 3(a-1)
\end{array}$$

since $n(z_5) = 2$ and $n(z_6) = 1$. Thus,

$$\begin{aligned}
\delta_4(a,b,1) \;&=\; \binom{a-3}{2} + \binom{a+b-3}{2} - \binom{a}{2} + (3a-8) \\
&\quad +(3a-2) + (6a-9) + (3a-5) + (3a-3).
\end{aligned}$$

Denote $P = \delta_4(a,b,1) - \delta_0(a,b,2)$. By Lemma 2.2 we have $\delta_0(a,b,2) = \binom{a+b+1}{2} + \binom{a+3}{2} - \binom{a+1}{2}$. Expanding the terms we get

$$P = 9a - 4b - 18.$$

Since $a \geq b$, we have $P \geq 5a - 18$, and as $a \geq 4$, we have $P \geq 0$. Since $\delta_4(a,b,2) \geq \delta_4(a,b,1)$ and $\delta_0(a,b,2) \geq \delta_0(a,b,1)$, we conclude $\delta_4(a,b,i) - \delta_0(a,b,i) \geq P \geq 0$ for $i \in \{1,2\}$.

Case 3. *$a \geq 4$, $b = 2$ and $c \leq 2$.*

We find $\delta_4(a,2,1)$. In $L^2(C_{a,2,1})$ we have $S_2 = S_3 = 0$. Again, the vertex z_3 is not defined here, $\deg(z_2) = 2$ and $\deg(z_5) = \deg(z_6) = 3$ (see Figure 2). Analogously as in the previous cases we get:

$$\begin{array}{ll}
S_1 = \binom{a-3}{2} & h(z_4) = 6(a-2)+3 \\
h(z_1) = 3(a-3)+1 & h(z_5) = 3(a-2)+1 \\
h(z_2) = (a-1) & h(z_6) = 3(a-1)
\end{array}$$

since $n(z_2) = 1$, $n(z_5) = 2$ and $n(z_6) = 1$. Thus,

$$\delta_4(a,2,1) = \binom{a-3}{2} + (3a-8) + (a-1) + (6a-9) + (3a-5) + (3a-3).$$

Denote $P = \delta_4(a,2,1) - \delta_0(a,2,2)$. By Lemma 2.2 we have $\delta_0(a,2,2) = 2\binom{a+3}{2} - \binom{a+1}{2}$. Expanding the terms we get

$$P = 8a - 26.$$

Since $a \geq 4$, we have $P \geq 0$. Since $\delta_4(a,2,2) \geq \delta_4(a,2,1)$ and $\delta_0(a,2,2) \geq \delta_0(a,2,1)$, we conclude $\delta_4(a,2,i) - \delta_0(a,2,i) \geq P \geq 0$ for $i \in \{1,2\}$.

Case 4. *$a \geq 4$ and $b = c = 1$.*

In $L^2(C_{a,1,1})$ we have $S_2 = S_3 = 0$. Note that the vertices z_2 and z_3 are not defined, while $\deg(z_4) = \deg(z_5) = 3$ and $\deg(z_6) = 2$ (see Figure 2). Analogously as in the previous cases we get:

$$\begin{array}{ll} S_1 = \binom{a-3}{2} & h(z_4) = h(z_5) = 3(a-2) + 1 \\ h(z_1) = 3(a-3) + 1 & h(z_6) = (a-1) \end{array}$$

since $n(z_4) = n(z_5) = 2$ and $n(z_6) = 0$. Thus,

$$\delta_4(a, 1, 1) = \binom{a-3}{2} + (3a-8) + 2(3a-5) + (a-1).$$

Denote $P = \delta_4(a, 1, 1) - \delta_0(a, 1, 1)$. By Lemma 2.2 we have $\delta_0(a, 1, 1) = 2\binom{a+2}{2} - \binom{a+1}{2}$. Expanding the terms we get

$$P = 4a - 15.$$

Since $a \geq 4$, we have $P \geq 0$, and hence $\delta_4(a, 1, 1) - \delta_0(a, 1, 1) \geq P \geq 0$. $\square$

Proof of Theorem 1.6. Let T be the tree $C_{a,b,c}$ with $a \geq b \geq c \geq 1$, such that $a \neq 1$. If $a \leq 3$, then $\Delta C_{a,b,c} = W(L^4(C_{a,b,c})) - W(C_{a,b,c}) > 0$, by Lemma 2.1.

Now suppose that $a \geq 4$. Consider lexicographical ordering of triples (a', b', c') with $a' \geq b' \geq c' \geq 1$ and $a' \geq 2$. Further, assume that $\Delta C_{a',b',c'} > 0$ for every triple (a', b', c'), such that $a' \geq b' \geq c' \geq 1$ and $a' \geq 2$, which is in the lexicographical ordering smaller than (a, b, c).

Let (a^*, b^*, c^*) be ordering of triple $(a-1, b, c)$, such that the multisets $\{a^*, b^*, c^*\}$ and $\{a-1, b, c\}$ are the same and $a^* \geq b^* \geq c^*$. Then $C_{a-1,b,c}$ and C_{a^*,b^*,c^*} are isomorphic graphs. Moreover, since $a \geq 4$, we have $a^* \geq 3$. By (1) and Lemma 2.5 we see that

$$\begin{aligned} \Delta C_{a,b,c} - \Delta C_{a^*,b^*,c^*} &= \Delta C_{a,b,c} - \Delta C_{a-1,b,c} \\ &= \delta_4(a, b, c) - \delta_0(a, b, c) \\ &\geq 0. \end{aligned}$$

Since (a^*, b^*, c^*) is in the lexicographical ordering smaller than (a, b, c) and $a^* \geq 2$, by the induction hypothesis we have $\Delta C_{a^*,b^*,c^*} > 0$. Hence, $\Delta C_{a,b,c} = W(L^4(C_{a,b,c})) - W(C_{a,b,c}) > 0$. $\square$

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