Bicyclic graphs with the second up to seventh largest Wiener indices*

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Abstract

The Wiener index of a connected graph is the sum of distances between all pairs of vertices in the graph. Feng et al. in [The hyper-Wiener index of bicyclic graphs, Utilitas Math., 84(2011) 97-104] determined the bicyclic graphs having the largest Wiener index. In this article we determine the graphs having the second up to seventh largest Wiener indices among all bicyclic graphs with n vertices.

Key words: Wiener index, bicyclic graph, pendant, transformation
AMS Classifications: 05C12, 05C90, 92E10

1. Introduction

All graphs considered in this paper will be finite, simple and undirected. Let G be a connected graph with vertex set $V(G)$ and let $deg_G(v)$ be the degree of a vertex v in G. The *distance* $d_G(u,v)$ between vertices u and v is the number of edges on a shortest path connecting these vertices in G. The distance $W(G,v)$ of a vertex $v \in V(G)$ is the sum of distances between v and all other vertices of G. Throughout the paper, for convenience, set $d_G(u,u) = 0$ and

$$f(x,k,l) = \frac{1}{6}(x^3 - kx + l).$$

The *Wiener index* $W(G)$ of a connected graph G is a graph invariant based on distances [1,2] and is the oldest topological index related to molecular branching [3]. It is defined to be the sum of distances between all pairs of vertices in G, i.e.,

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v) = \frac{1}{2} \sum_{v \in V(G)} W(G,v).$$

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A quantity closely related to $W(G)$ is the *average distance* $\mu(G)$ that is defined by

$$\mu(G) = \frac{W(G)}{\binom{|G|}{2}},$$

where $|G|$ is the number of vertices of G. If G represents a network (e.g., an interconnection network connecting many processors) then $\mu(G)$ is the average distance between the nodes (or processors) of the network. So it is a measure of the average delay of messages for traversing from one node to another. It is obvious that studying $\mu(G)$ is equivalent to studying $W(G)$.

For trees and hexagonal systems, the study of Wiener index has made the greatest progress (see two surveys [4,5]). In particular, for trees many researchers investigated the relations of Wiener index and some isomorphic invariants of graphs, such as maximum degree, diameter, degree sequence, independence number, domination number, et al. (see, e.g., [6-12]).

Except trees, some results of Wiener index on the other graphs were also obtained. For example, Wiener [1] obtained the largest and smallest Wiener index of unicyclic graphs. Tang and Deng [13] identified the graphs having the first three smaller and larger Wiener indices among all unicyclic graphs. Du and Zhou [14] determined the graphs having the smallest Wiener index among all unicyclic graphs given matching number. Yu and Feng [15] investigated the Wiener index of unicyclic graphs given girth. Tang and Deng [16] determined the smallest Wiener index of bicyclic graphs. Feng et al. [17] identified the unique graph having the largest Wiener index among all bicyclic graphs. Tan and Wang [18] characterized the graphs having the smallest Wiener index among all cacti given cycle number and matching number. Dankelmann [19,20] determined the maximum Wiener index of a connected graph given independence number or domination number. Tomescu and Melter [21] determined the minimum and maximum Wiener index of a connected graph given chromatic number.

A *bicyclic graph* is a connected graph in which its number of edges equals its number of vertices plus one. The *base* $\hat{G}$ of a bicyclic graph G is the minimal bicyclic subgraph of G. Bases of bicyclic graphs have two types: $B_1(p,s,q)$ and $B_2(p,s,q)$ (see Fig. 1). From the bases of bicyclic graphs, it is obvious that the set $B(n)$ of n-vertex bicyclic graphs can be partitioned into two subsets $B_1(n)$ and $B_2(n)$, respectively, as follows:

$$B_1(n) = \{G \in B(n) : \text{there exist three integers } p \geq 3,\ q \geq 3 \text{ and } s \geq 1 \text{ such that } \hat{G} \cong B_1(p,s,q)\}.$$

$$B_2(n) = \{G \in B(n) : \text{there exist three integers } p \geq 1,\ q \geq 1 \text{ and } s \geq 0 \text{ such that } \hat{G} \cong B_2(p,s,q)\}.$$

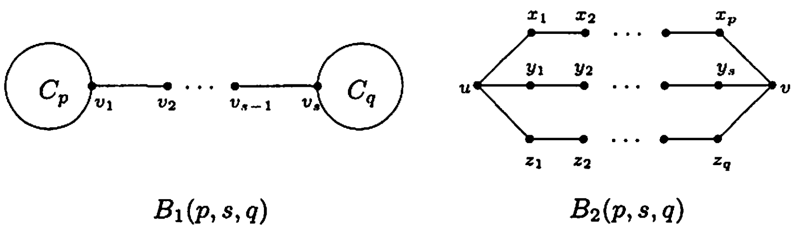


Fig. 1 Two bases of bicyclic graphs

Motivated by the results above, especially [13-17], in this article we present some graphic transformations and characterize the graphs having the second up to seventh largest Wiener indices among all bicyclic graphs.

The rest of the work is organized as follows. In Section 2 we present some new and useful transformations of graphs that change the Wiener index of graphs. In Section 3 we determine the graphs having the second and third largest Wiener indices in $B_1(n)$. In Section 4 we characterize the graphs having the second up to sixth largest Wiener indices in $B_2(n)$. In Section 5 we determine the graphs with the second up to seventh largest Wiener indices among all n-vertex bicyclic graphs for $n \geq 10$.

2. The Wiener index of graphs under transformations

In this section we give some new and useful transformations of graphs that change the Wiener index of graphs, which will be used in the sequel.

Lemma 2.1 [22]. *Let G be a connected graph with a cut-vertex u, and let G_1 and G_2 be two connected subgraphs of G such that $V(G_1) \bigcap V(G_2) = \{u\}$ and $G_1 \bigcup G_2 = G$. Then*

$$W(G) = W(G_1) + W(G_2) + (|G_1| - 1)W(G_2, u) + (|G_2| - 1)W(G_1, u).$$

For three connected graphs G_1, G_2 and G_3, let v, x and y be vertices of G_1, G_2 and G_3, respectively. Let $Q(G_1, G_2, s)$ be the graph obtained from G_1 and G_2 by joining v to x with a path $v_1 v_2 \cdots v_s$ in which $v_1 = v$ and $v_s = x$. Let G be the graph obtained from $Q(G_1, G_2, s)$ and G_3 by identifying y and v_i $(1 \leq i \leq s)$, while let G' be another graph obtained from $Q(G_1, G_2, s)$ and G_3 by identifying y and a vertex u of G_1 distinct from v.

Theorem 2.2. *Let G and G' be the two graphs defined above with $|G_2| \geq |G_1| \geq 2$ and $|G_3| \geq 2$. If $W(G_1, u) \geq W(G_1, v)$, then $W(G') > W(G)$.*

Proof. Set $Q = Q(G_1, G_2, s)$ and $d_{G_1}(u, v) = r$. By Lemma 2.1 we have

$$W(G) = W(G_3) + W(Q) + (|G_3| - 1)W(Q, v_i) + (|Q| - 1)W(G_3, y). \quad (2.1)$$

$$W(G') = W(G_3) + W(Q) + (|G_3|-1)W(Q,u) + (|Q|-1)W(G_3,y). \quad (2.2)$$

Note that

$$W(Q,v_i) = W(G_1,v) + |G_1|(i-1) + \sum_{j=1}^{i-2} j + W(G_2,x) + |G_2|(s-i) + \sum_{j=1}^{s-1-i} j,$$

$$W(Q,u) = W(G_1,u) + \sum_{j=1}^{s-2}(r+j) + W(G_2,x) + |G_2|(r+s-1),$$

so we get that

$$W(Q,u) - W(Q,v_i) = [W(G_1,u) - W(G_1,v)] + (s-1)r + (i-1)(s-i)$$
$$+(|G_2| - |G_1|)(i-1) + r(|G_2|-1) > 0.$$

Therefore, by Eqs. (2.1) and (2.2) it follows that

$$W(G') - W(G) = (|G_3|-1)[W(Q,u) - W(Q,v_i)] > 0.$$

This proof is complete. □

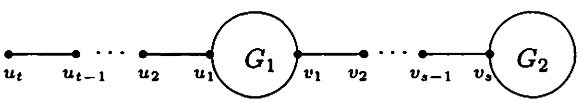


Fig. 2 $G(G_1, G_2, s, t)$

Theorem 2.3. *Let G_1 and G_2 be two arbitrary connected graphs, and let u and v be two arbitrary vertices (maybe same) of G_1 such that $|G_1| > d_{G_1}(u,v) + 1$. Let $G(G_1, G_2, s, t)$ be the graph obtained from G_1 and G_2 by adding a path $u_1u_2\cdots u_t$ to the vertex u and joining the vertex v to a vertex x of G_2 with a path $v_1v_2\cdots v_s$ in which $u_1 = u$, $v_1 = v$ and $v_s = x$ (see Fig. 2). If $W(G_1,v) \geq W(G_1,u)$ and $k > \max\{0, t+1-s-|G_2|\}$, then we have that*

$$W(G(G_1,G_2,s+k,t-k)) > W(G(G_1,G_2,s,t)).$$

Proof. Let H_1 and H_2 be the two graphs obtained from G_1 and G_2 by attaching paths $u_1u_2\cdots u_t$ and $v_1v_2\cdots v_s$ at u and x, respectively, where $u_1 = u$ and $v_s = x$. Write

$$G(s,t) = G(G_1,G_2,s,t), \quad p = |G_1| + t - 2, \quad q = |G_2| + s - 2.$$

By Lemma 2.1 we have that

$$W(G(s,t)) = W(H_1) + W(H_2) + pW(H_2,v_1) + qW(H_1,v). \qquad (2.3)$$

It is obvious that $G(s+k,t-k)$ is isomorphic to the graph F obtained from $G(s,t)$ by deleting $u_t, u_{t-1}, \cdots, u_{t-k+1}$ and inserting k new vertices $\bar{v}_1, \bar{v}_2, \cdots, \bar{v}_k$ of degree two into the edge v_1v_2. Let Q_1 and Q_2 be the graphs containing $\bar{v}_k$ in $F-\bar{v}_kv_2$ and $F-\bar{v}_{k-1}\bar{v}_k$, respectively. Then

$$V(Q_1)\bigcap V(Q_2)=\{\bar{v}_k\},\ \ Q_1\bigcup Q_2=F.$$

So by Lemma 2.1 it follows that

$$W(G(s+k,t-k))=W(Q_1)+W(Q_2)+pW(Q_2,\bar{v}_k)+qW(Q_1,\bar{v}_k). \quad (2.4)$$

Since $Q_2\cong H_2$ and $\bar{v}_k$ is the vertex of Q_2 corresponding to the vertex v_1 of H_2, it follows that $W(Q_2)=W(H_2)$ and $W(Q_2,\bar{v}_k)=W(H_2,v_1)$. Set

$$\Delta=W(G(s+k,t-k))-G(s,t),$$

then by Eqs. (2.3) and (2.4) we get that

$$\Delta=[W(Q_1)-W(H_1)]+q[W(Q_1,\bar{v}_k)-W(H_1,v)] \quad (2.5)$$

Write $r=d_{G_1}(u,v)$ and write

$$P=u_tu_{t-1}\cdots u_{t-k},\ \ \bar{P}=v\bar{v}_1\cdots\bar{v}_k,\ \ Z=H_1-\{u_t,u_{t-1},\cdots,u_{t-k+1}\}.$$

Then again by Lemma 2.1 we have that

$$W(H_1)=W(Z)+W(P)+(p-k)W(P,u_{t-k})+kW(Z,u_{t-k}).$$

$$W(Q_1)=W(Z)+W(\bar{P})+(p-k)W(\bar{P},v)+kW(Z,v).$$

Therefore, from $P\cong\bar{P}$ and $W(P,u_{t-k})=W(\bar{P},v)$ we get that

$$W(Q_1)-W(H_1)=k[W(Z,v)-W(Z,u_{t-k})]$$

$$=k\{[W(G_1,v)+\sum_{j=1}^{t-k-1}(r+j)]-[W(G_1,u)+(t-k-1)|G_1|+\sum_{j=1}^{t-k-2}j]\}$$

$$=k[W(G_1,v)-W(G_1,u)]-k(t-k-1)(|G_1|-r-1)]. \quad (2.6)$$

On the other hand, it is easy to see that

$$W(H_1,v)=W(G_1,v)+\sum_{j=1}^{t-1}(r+j).$$

$$W(Q_1,\bar{v}_k)=\sum_{j=1}^{t-k-1}(r+k+j)+W(G_1,v)+k|G_1|+\sum_{j=1}^{k-1}j.$$

Therefore, it follows that

$$W(Q_1, \bar{v}_k) - W(H_1, v) = k(|G_1| - r - 1). \tag{2.7}$$

Write $\mu = s - t - 1$. Note that $q = |G_2| + s - 2$ and $r = d_{G_1}(u, v)$, so by Eqs. (2.5)-(2.7) we have that

$$\Delta = k[W(G_1, v) - W(G_1, u)] + k(k + |G_2| + \mu)(|G_1| - d_{G_1}(u, v) - 1). \tag{2.8}$$

Hence by the assumptions we have $\Delta > 0$. This proof is complete. □

Corollary 2.4. *Let u and v be two arbitrary nonpendant vertices (maybe same) of a connected graph M. Let $M_{s,t}$ be the graph obtained from M by adding two paths $u_1u_2\cdots u_s$ and $v_1v_2\cdots v_t$ to u and v, respectively, where $u_1 = u$, $v_1 = v$. If $s \geq 2$ and $t \geq 2$, then we have that*

$$W(M_{s+t-1,1}) > W(M_{s,t}) \quad or \quad W(M_{1,s+t-1}) > W(M_{s,t}).$$

Proof. Assume that $W(M, v) \geq W(M, u)$. Now we only need to prove $W(M_{0,s+t}) > W(M_{s,t})$. In Theorem 2.3, set $G_1 = M$ and $G_2 = v_s$. Then

$$M_{s,t} \cong G(M, v_s, s, t), \quad M_{1,s+t-1} \cong G(M, v_1, s + t - 1, 1).$$

Since u, v are nonpendant vertices of M and $s \geq 2$, it follows that

$$|M| > d_M(u, v) + 1, \quad t - 1 > \max\{0, t + 1 - s - |G_2|\}.$$

Therefore, by taking $k = t - 1$ in Theorem 2.3 we get that

$$W(M_{1,s+t-1}) = W(G(M, v_1, s + t - 1, 1)) > W(G(M, v_1, s, t)) = W(M_{s,t}).$$

In a similar way, when $W(M, u) \geq W(M, v)$, we can also prove that

$$W(M_{s+t-1,1}) > W(M_{s,t}).$$

This proof is complete. □

Corollary 2.5. *Let uv be an edge of a connected graph N with $deg_N(u) \geq 2$ and let $N_{s,t}$ be the graph obtained from N by attaching two vertex-disjoint paths $u_1u_2\cdots u_s$ and $v_1v_2\cdots v_t$ at u and v, respectively, where $u_1 = u$ and $v_1 = v$. If $s \geq t \geq 2$, then we have that*

$$W(N_{s+1,t-1}) > W(N_{s,t}).$$

Proof. In Theorem 2.3, set $G_1 = N$ and $G_2 = v_s$. Then $N_{s,t} \cong G(N, v_s, s, t)$. So by taking $k = 1$ and $d_N(u, v) = 1$ in Eq. (2.8), we get that

$$W(N_{s+1,t-1}) - W(N_{s,t}) = W(N, v) - W(N, u) + (s + 1 - t)(|N| - 2). \tag{2.9}$$

We partition $V(N)$ into the three subsets V_1, V_2, V_3 as follows:

$$V_1 = \{z : z \in V(N),\ \ d_N(z,u) < d_N(z,v)\},$$
$$V_2 = \{z : z \in V(N),\ \ d_N(z,u) > d_N(z,v)\},$$
$$V_3 = \{z : z \in V(N),\ \ d_N(z,u) = d_N(z,v)\}.$$

Then we get that

$$W(N,u) = \sum_{z\in V_1} d_N(z,u) + \sum_{z\in V_2} [d_N(z,v)+1] + \sum_{z\in V_3} d_N(z,u)$$

$$W(N,v) = \sum_{z\in V_1} [d_N(z,u)+1] + \sum_{z\in V_2} d_N(z,v) + \sum_{z\in V_3} d_N(z,v).$$

It follows that

$$W(N,v) - W(N,u) = |V_1| - |V_2|. \tag{2.10}$$

Write $a = s - t \geq 0$. Then by $|N| = |V_1| + |V_2| + |V_3|$ and Eqs. (2.9)-(2.10) we get that

$$\begin{aligned} W(N_{s+1,t-1}) - W(N_{s,t}) &= |V_1| - |V_2| + (s+1-t)(|V_1| + |V_2| + |V_3| - 2) \\ &= (a+2)(|V_1|-2) + a|V_2| + (a+1)|V_3| + 2. \quad (2.11) \end{aligned}$$

From $deg_N(u) \geq 2$ we see that $|V_1| \geq 2$. So by Eq. (2.11) it follows that

$$W(N_{s+1,t-1}) - W(N_{s,t}) \geq 2 > 0.$$

This proof is complete. □

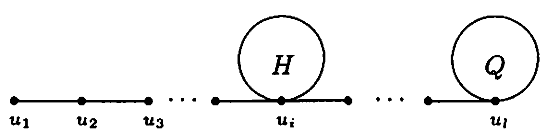


Fig. 3 $QH(l,i)$

Corollary 2.6. *Let Q and H be two connected graphs with $|Q| \geq 2$ and $|H| \geq 2$. Let $QH(l,i)$ denote the graph obtained from Q, H and a path $u_1u_2\cdots u_l (l \geq 2)$ by identifying a vertex v of H and u_i, and identifying a vertex x of Q and u_l (still denote the two new vertices by u_i and u_l, respectively) (see Fig. 3). If $1 \leq j < \min\{i, |Q|+l-i\}$, then we have that*

$$W(QH(l,j)) > W(QH(l,i)).$$

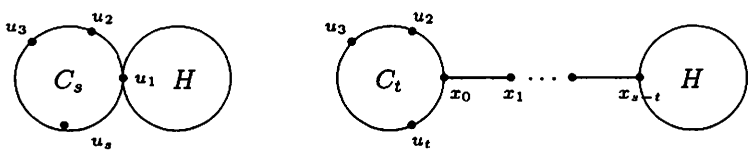
Proof. In Theorem 2.3, take

$$u = v,\ \ G_1 = H,\ \ G_2 = Q,\ \ t = i,\ \ s = l - i + 1,\ \ k = i - j.$$

Then $QH(l,i) \cong G(H,Q,i,\mu+1)$ in which $\mu = l-i$. By Eq. (2.8) we have

$$W(QH(l,j))-W(QH(l,i)) = W(G(H,Q,j,l-j+1))-W(G(H,Q,i,\mu+1))$$
$$= (|H|-1)(i-j)(|Q|+l-i-j) > 0.$$

This proof is complete. □



$G(H,s)$ $G(H,s,t)$

Fig. 4

Let u be a vertex of a connected graph H. Let $G(H,s)$ be the graph obtained from H and a cycle $C_s = u_1u_2\cdots u_su_1$ by identifying u and u_1, while let $G(H,s,t)$ be the other graph obtained from H and a cycle $C_t = u_1u_2\cdots u_tu_1$ by joining u_1 to u with a path $x_0x_1x_2\cdots x_{s-t}$ in which $x_0 = u_1$ and $x_{s-t} = u$ (see Fig. 4). In particular, the transformation from $G(H,s)$ to $G(H,s,3)$ has been studied in [17]. It is known that

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

Theorem 2.7. *Let $G(H,s)$ and $G(H,s,t)$ be the two graphs defined above such that $|H| \geq 2$ and $s \geq t+1$. Then for $3 \leq t \leq 6$, we have that*

$$W(G(H,s,t)) > W(G(H,s)).$$

Proof. Write $\theta = |H|-1$. By Lemma 2.1 we have that

$$W(G(H,s)) = W(C_s) + W(H) + (s-1)W(H,u) + \theta W(C_s,u_1). \quad (2.12)$$

Let Q denote the vertex-induced subgraph of $\{u_2,u_3,\cdots,u_t,x_0,x_1,\cdots,x_{s-t}\}$ in $G(H,s,t)$. Then

$$W(G(H,s,t)) = W(Q) + W(H) + (s-1)W(H,u) + \theta W(Q,x_{s-t}). \quad (2.13)$$

Write $P_{s-t+1} = x_0x_1x_2\cdots x_{s-t}$. Then

$$W(Q) = W(C_t) + W(P_{s-t+1}) + (t-1)W(P_{s-t+1},x_0) + (s-t)W(C_t,u_1)$$

$$= \frac{(2s-t)W(C_t)}{t} + \binom{s-t+2}{3} + \frac{(s-t)(s-t+1)(t-1)}{2}$$

$$= \frac{(2s-t)W(C_t)}{t} + \frac{(s-t)(s-t+1)(s+2t-1)}{6}. \tag{2.14}$$

By a straightforward calculation we have that

$$W(Q, x_{s-t}) = W(C_t, u_1) + t(s-t) + \frac{(s-t)(s-t-1)}{2}$$

$$= \frac{2W(C_t)}{t} + \frac{(s-t)(s+t-1)}{2}. \tag{2.15}$$

Write $\Delta(s,t) = W(G(H,s,t)) - W(G(H,s))$ and $\delta = s-t$. Then from Eqs. (2.12)-(2.15) it follows that

$$\begin{aligned}\Delta(s,t) &= [W(Q) - W(C_s)] + \theta[W(Q, x_{s-t}) - W(C_s, u_1)] \\ &= \frac{(2s-t)W(C_t)}{t} + \frac{(s-t)(s-t+1)(s+2t-1)}{6} - W(C_s) \\ &+\theta[\frac{2W(C_t)}{t} + \frac{(s-t)(s+t-1)}{2} - \frac{2W(C_s)}{s}] \\ &\geq \frac{(2s-t)(t^2-1)}{8} + \frac{(s-t)(s-t+1)(s+2t-1)}{6} - \frac{s^3}{8} \\ &+\theta[\frac{t^2-1}{4} + \frac{(s-t)(s+t-1)}{2} - \frac{s^2}{4}] \\ &= \frac{1}{24}[\delta(s^2+st-5t^2+12t-7) - 3s] + \frac{1}{4}[\delta(s+t-2) - 1]\theta \\ &\geq \frac{1}{24}[(s-t)(s^2+st-5t^2+6s+18t-19) - 3s - 6].\end{aligned}$$

So for $3 \leq t \leq 6$, by the last equation it is easy to see that $\Delta(s,t) > 0$. □

Theorem 2.8. *Let u, v be two distinct vertices of a connected graph G and let x be a vertex of a non-trivial connected graph H. Let $G(u,H)$ denote the graph formed from G and H by identifying u and x. If $W(G,u) > W(G,v)$, then we have that*

$$W(G(u,H)) > W(G(v,H)).$$

Proof. By Lemma 2.1 we have that

$$W(G(u,H)) = W(G) + W(H) + (|G|-1)W(H,x) + (|H|-1)W(G,u).$$

$$W(G(v,H)) = W(G) + W(H) + (|G|-1)W(H,x) + (|H|-1)W(G,v).$$

Therefore, it follows that

$$W(G(u,H)) - W(G(v,H)) = (|H|-1)[W(G,u) - W(G,v)] > 0.$$

This proof is complete. □

3. The graphs with larger Wiener indices in $B_1(n)$

In [16], the authors had proved that $B_1(3, n-4, 3)$ is the unique graph with the largest Wiener index in $B_1(n)$. In the section we further characterize all graphs with the second and third largest Wiener indices in $B_1(n)$.

In a connected graph G, a *pendant vertex* is a vertex of degree one and a pendant edge is an edge incident to a pendant vertex. Let $P = u_0u_1u_2\cdots u_k$ be a path of G with distinct vertices $u_0, u_1, \cdots, u_k$. If

$$deg_G(u_0) \geq 3,\ deg_G(u_1) = \cdots = deg_G(u_{k-1}) = 2,\ deg_G(u_k) = 1,$$

then P is called a *pendant path* of length k at u_1 in G.

Lemma 3.1. *Let H be a n-vertex connected graphs with at least two pendant paths. Then there exists a n-vertex connected graph Q with a unique pendant path such that $W(H) < W(Q)$.*

Proof. Assume that $uu_1u_2\cdots u_k$ and $vv_1v_2\cdots v_l$ are two pendant paths of H, respectively, at vertices u and v. From Corollary 2.4 we have that

$$W(H) < W(H - vv_1 + u_kv_1) \text{ or } W(H) < W(H - uu_1 + v_lu_1).$$

If $W(H) < W(H - vv_1 + u_kv_1)$, then set $H_1 = H - vv_1 + u_kv_1$, and set $H_1 = H - uu_1 + v_lu_1$ otherwise. It is obvious that the number of pendant paths of H_1 is less than that of H. If H_1 still contains two pendant paths, then to H_1 repeat the above procedure until we get a n-vertex connected graph H_r such that it contains a unique pendant path. So we obtain some n-vertex connected graphs $H, H_1, \cdots, H_\xi$ such that

$$W(H) < W(H_1) < \cdots < W(H_\xi).$$

By taking $Q = H_\xi$, we arrive at the required result. $\square$

By Lemma 2.1, by a straightforward calculation we get that

$$W(B_1(p,s,q)) = W(C_p)[1 + \frac{2(s+q-2)}{p}] + W(C_q)[1 + \frac{2(s+p-2)}{q}]$$

$$+ \binom{s+1}{3} + \frac{1}{2}(s-1)[(s-2)(p+q-2) + 2(pq-1)]. \quad (3.1)$$

From Eq. (3.1) we easily get that

$$W(B_1(3, n-4, 3)) = f(n, 13, 24). \quad (3.2)$$

$$W(B_1(4, n-5, 3)) = f(n, 19, 48). \quad (3.3)$$

Now denote the two cycles of $B_1(p, s, q)$ by

$$C_p = v_1a_2a_3\cdots a_pv_1,\quad C_q = v_sb_2b_3\cdots b_qv_s.$$

Let $H(p,s,q,t,i)$ be the graph obtained from $B_1(p,s,q)$ by adding a pendant path $a'_1a'_2a'_3\cdots a'_t$ to a_i in which $a'_1 = a_i$ $(2 \le i \le \lceil \frac{p+1}{2} \rceil)$. By Lemma 2.1 and Eq. (3.2) it is easy to get that

$$W(H(3,n-5,3,2,2)) = f(n,19,48). \tag{3.4}$$

$$W(H(3,n-6,3,3,2)) = W(H(3,1,3,n-4,2)) = f(n,25,84). \tag{3.5}$$

In the following of this section, we always assume that $n \ge 7$ and

$$B \in B_1(n) - \{B_1(3,n-4,3), B_1(4,n-5,3), H(3,n-5,3,2,2),$$
$$H(3,n-6,3,3,2), H(3,1,3,n-4,2)\}. \tag{3.6}$$

Lemma 3.2. *If B has not pendant paths, then $W(B) < f(n,25,84)$.*
Proof. Now there are integers $p \ge 3$, $q \ge 3$ and $s \ge 1$ with $p+s+q = n+2$ such that $B = B_1(p,s,q)$. From Eq. (3.6), especially $B \notin \{B_1(3,n-4,3), B_1(4,n-5,3)\}$, we see that $p+q \ge 8$. Assume, without loss of generality, that $p \ge q$. Then $q = 3$ and $p \ge 5$ or $q \ge 4$. Thus we may distinguish the two following cases.
Case 1 Assume that $q = 3$ and $p \ge 5$.
By taking the vertex-induced subgraph of $\{v_1, v_2, \cdots, v_s, b_2, \cdots, b_q\}$ in B as H in Theorem 2.8, then from Theorem 2.8 we get that

$$W(B) = W(G(H,p)) \le W(G(H,s,5)) = W(B_1(5,n-6,3)). \tag{3.7}$$

By Eq. (3.1) we easily see that $W(B_1(5,n-6,3)) = f(n,31,102)$. So by Eq. (3.7) it follows that $W(B) < f(n,25,84)$.
Case 2 Assume that $q \ge 4$.
If $p = 4$, then $B = B_1(4,n-6,4)$. From Eq. (3.1) we have that

$$W(B) = W(B_1(4,n-6,4)) = f(n,25,72) < f(n,25,84).$$

Next assume that $p \ge 5$. By taking the vertex-induced subgraph of $\{v_1, \cdots, v_s, a_2, \cdots, a_p\}$ in B as H in Theorem 2.8, then from Theorem 2.8 we get that

$$W(B) = W(G(H,q)) < W(G(H,q,3)) = W(B_1(p,n-p-1,3)). \tag{3.8}$$

By the result of Case 1 we have that $W(B_1(p,n-p-1,3)) < f(n,25,84)$. Thus by Eq. (3.8) it follows that $W(B) < f(n,25,84)$. □
Lemma 3.3. *If B has pendant paths, then $W(B) < f(n,25,84)$.*
Proof. There are integers $p \ge 3$, $q \ge 3$ and $s \ge 1$ such that $\hat{B} = B_1(p,s,q)$. By Lemma 3.1 there exists a connected graph Q that contains a unique pendant path of length $t-1 = n-p-q-s+2 \ge 1$ and $\hat{Q} = \hat{B}$ such that

$$W(B) \le W(Q). \tag{3.9}$$

If the unique pendant path of Q is at some vertex of two cycles, say a_i in $\{a_2, \cdots, a_p\}$, then set $Q' = Q$. Otherwise, let Q' be the graph obtained from Q by moving the unique path of Q from $v_i (1 \le i \le s)$ to some vertex of two cycles, say a_i in $\{a_2, \cdots, a_p\}$. By Theorem 2.2 we have that

$$W(Q) \le W(Q'). \tag{3.10}$$

Now we distinguish the three following cases.

Case 1 Assume that $p + q \ge 8$.

Using the notation of Theorem 2.3, we have that $Q' = G(C_p, C_q, s, t)$. Since $p > d_{C_p}(a_i, v_1) + 1$ and $W(C_p, a_i) = W(C_p, v_1)$, by taking $k = t - 1$ in Theorem 2.3 it follows that

$$W(Q') < W(G(C_p, C_q, s + t - 1, 1)) = W(B_1(p, s + t - 1, q)). \tag{3.11}$$

Thus by Eqs. (3.9)-(3.11) and the result of Lemma 3.2 we get that

$$W(B) < W(B_1(p, s + t - 1, q)) < f(n, 25, 84).$$

Case 2 Assume that $p + q = 7$.

Using the notation of Theorem 2.3, we have that $Q' = G(C_p, C_q, s, t)$. Since $p > d_{C_p}(a_i, v_1) + 1$ and $W(C_p, a_i) = W(C_p, v_1)$, by taking $k = t - 2$ in Theorem 2.3 it follows that

$$W(Q') \le W(G(C_p, C_q, s + t - 2, 2)), \tag{3.12}$$

where if $p = 3$, then $G(C_p, C_q, s + t - 2, 2) = H(3, n - 6, 4, 2, 2)$; if $p = 4$, then

$$G(C_p, C_q, s + t - 2, 2) \in \{H(4, n - 6, 3, 2, 2),\ H(4, n - 6, 3, 2, 3)\}.$$

Write $Z = B_1(3, n - 6, 4)$. It is easy to see that

$$W(Z, b_3) = \frac{1}{2}(n - 3)(n - 2),\ \ W(Z, b_2) = \frac{1}{2}(n^2 - 7n + 16),$$

$$W(Z, a_2) = \frac{1}{2}(n - 4)(n - 1).$$

Thus $W(Z, b_3) > \max\{W(Z, a_2), W(Z, b_2)\}$. By Theorem 2.8 we have that

$$W(H(4, n{-}6, 3, 2, 3)) > \max\{W(H(3, n{-}6, 4, 2, 2)), W(H(4, n{-}6, 3, 2, 2))\}. \tag{3.13}$$

By Lemma 2.1 and Eq. (3.3) it is easy to get that

$$W(H(4, n - 6, 3, 2, 3)) = f(n, 25, 78).$$

By Eqs. (3.9), (3.10), (3.12) and (3.13), we get that $W(B) < f(n,25,84)$.

Case 3 Assume that $p+q=6$. We distinguish the two following cases.

Subcase 3.1 Assume that B contains at least two pendant paths.

At present the inequality in Eq. (3.9) is strict and $Q' = H(3,s,3,t,2)$, where $t \geq 3$ and $s+t = n-3$. By taking $k = t-3$ in Theorem 2.3 we get

$$W(H(3,s,3,t,2)) \leq W(H(3,s+t-3,3,3,2)) = f(n,25,84). \qquad (3.14)$$

Therefore, we get that

$$W(B) < W(Q) \leq W(Q') = W(H(3,s,3,t,2)) \leq f(n,25,84).$$

Subcase 3.2 Assume that B only contains a pendant path.

If the unique pendant path of B is at the vertices a_i or $b_i (i = 2,3)$, then $B = H(3,s,3,t,2)$ in which $s+t = n-3$. From Eq. (3.6), especially

$$B \notin \{B_1(3,n-4,3), H(3,n-5,3,2,2), H(3,n-6,3,3,2), H(3,1,3,n-4,2)\},$$

we see that $4 \leq t \leq n-5$. It follows that the inequality (3.14) is strict. So

$$W(B) = W(H(3,s,3,t,2)) < f(n,25,84).$$

If the unique pendant path of B is at some vertex v_i, then by applying the transformation defined in Corollary 2.6, B can be transformed into a graph L_j that is obtained from $B_1(3,n-5,3)$ by adding a pendant edge to some vertex v_j. Assume, without loss of generality, that $1 \leq j \leq \frac{n-5}{2}$. By Lemma 2.1 and Eq. (3.2) we get that

$$W(L_j) = W(B_1(3,n-5,3)) + (2n-5) + \frac{1}{2}j(j+1) + \frac{1}{2}(n-4-j)(n-3-j).$$

It is easy to see that $W(L_{j+1}) - W(L_j) = 2j-(n-5) < 0$ for $1 \leq j \leq \frac{n-5}{2}$. So

$$W(L_j) \leq W(L_1) = f(n,25,72) < f(n,25,84).$$

By Corollary 2.6, it follows that $W(B) \leq W(L_j) < f(n,25,84)$. □

From Eqs. (3.2)-(3.5) and Lemmas 3.2-3.3 we immediately get the main result in this section as follows.

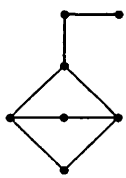
Theorem 3.4. *If $n \geq 7$ and B satisfies Eq. (3.6), then*

$$W(B) < W(H(3,n-6,3,3,2)) = W(H(3,1,3,n-4,2))$$

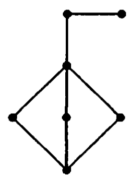
$$< W(B_1(4,n-5,3)) = W(H(3,n-5,3,2,2)) < W(B_1(3,n-4,3)).$$

4. The graphs with larger Wiener indices in $B_2(n)$

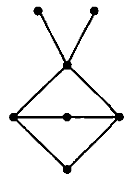
In [17], the authors had determined the unique graph having the largest Wiener index in $B_2(n)$. In this section we further characterize all graphs having the second up to sixth largest Wiener indices in $B_2(n)$.



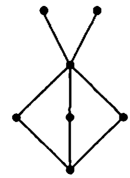
G_1



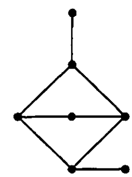
G_2



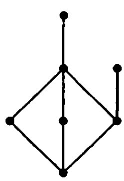
G_3



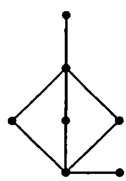
G_4



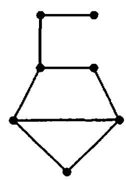
G_5



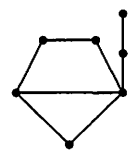
G_6



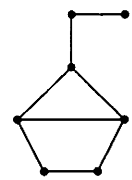
G_7



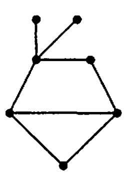
G_8



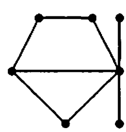
G_9



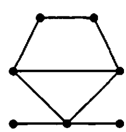
G_{10}



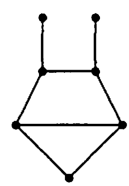
G_{11}



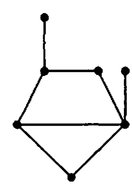
G_{12}



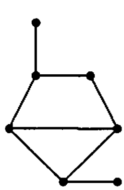
G_{13}



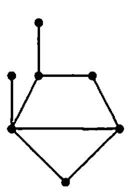
G_{14}



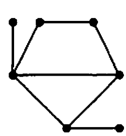
G_{15}



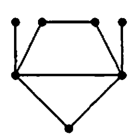
G_{16}



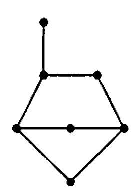
G_{17}



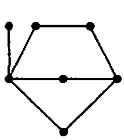
G_{18}



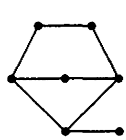
G_{19}



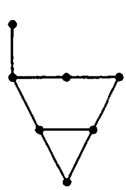
G_{20}



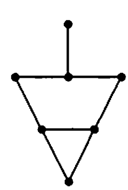
G_{21}



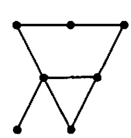
G_{22}



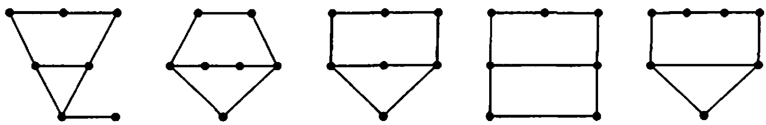
G_{23}



G_{24}



G_{25}



G_{26} G_{27} G_{28} G_{29} G_{30}

Fig. 5 All graphs in $B_2^1(7)$

In this section always write $B_2(1,0,1) = B_0$. Divide $B_2(n)$ into two subsets $B_2^1(n)$ and $B_2^2(n)$ as follows:

$$B_2^1(n) = \{G : G \in B_2(n), \hat{G} \ncong B_0\}, \quad B_2^2(n) = \{G : G \in B_2(n), \hat{G} \cong B_0\}.$$

Recall the labels of vertices of $B_2(p,s,q)$ in Fig. 1. For non-negative integers k,l,r,t, let $B_{r,t}^{k,l}$ be the n-vertex graph obtained from B_0 by adding four pendant paths of lengths r,t,k,l to the vertices u, v, x_1, y_1, respectively. Let u be a vertex of a connected graph G and let $G(u,\delta,\theta,\eta)$ be the n-vertex graph obtained from G by adding a path $u_1u_2\cdots u_\delta$ to u in which $u = u_1$, then adding two paths $u_\delta a_1 a_2 \cdots a_\theta$ and $u_\delta b_1 b_2 \cdots b_\eta$ to u_δ. Set

$$F_1(n) = B_{0,0}^{n-4,0}, \quad F_2(n) = B_{0,0}^{n-5,1}, \quad F_3(n) = B_{n-4,0}^{0,0},$$

$$F_4(n) = B_0(x_1, n-5, 1, 1), \quad F_5(n) = B_{0,0}^{n-6,2}, \quad F_6(n) = B_{1,0}^{n-5,0}.$$

Let $F_7(n)$ be the graph obtained from $B_2(1,1,1)$ by adding a pendant path of length $n-5$ to the vertex x_1. Let $F_8(n)$ and $F_9(n)$ be the two graphs obtained from $B_2(2,0,1)$ by adding a pendant path of length $n-5$ to the vertices x_1 and z_1, respectively. From Lemma 2.1, by a straightforward calculation we get that

$$W(F_1(n)) = f(n, 13, 30). \tag{4.1}$$

$$W(F_2(n)) = f(n, 19, 60). \tag{4.2}$$

$$W(F_3(n)) = f(n, 19, 54). \tag{4.3}$$

$$W(F_4(n)) = f(n, 19, 48). \tag{4.4}$$

$$W(F_5(n)) = f(n, 25, 102). \tag{4.5}$$

$$W(F_6(n)) = W(F_7(n)) = W(F_8(n)) = W(F_9(n)) = f(n, 25, 84). \tag{4.6}$$

$$W(B_0(x_1, n-6, 2, 1)) = W(B_{0,0}^{0,1}(x_1, n-6, 1, 1)) = f(n, 25, 78). \tag{4.7}$$

$$W(B_0(u, n-5, 1, 1)) = f(n, 25, 72). \tag{4.8}$$

$$W(B_{0,0}^{n-7,3}) = f(n,31,156). \tag{4.9}$$

$$W(B_{n-5,0}^{1,0}) = f(n,31,120). \tag{4.10}$$

Lemma 4.1. *If $n \geq 7$, then for $B \in B_2^1(n)$ and any vertex v of B we have*

$$W(B,v) \leq \frac{1}{2}(n^2 - n - 8), \tag{4.11}$$

with equality if and only if $B \in \{F_7(n), F_8(n), F_9(n)\}$ and v is the unique pendant vertex of B.

Proof. If v is not a pendant vertex of B, then in [17] it has been proved that $W(B,v) \leq \frac{1}{2}n^2 - \frac{3}{2}n + 2$. Therefore, we get that

$$W(B,v) \leq \frac{1}{2}n^2 - \frac{3}{2}n + 2 < \frac{1}{2}(n^2 - n - 8).$$

Next assume that v is a pendant vertex of B. Now we prove Eq. (4.11) by induction on $n \geq 7$.

When $n = 7$, all graphs in $B_2^1(7)$ have been shown in Fig. 5, where $G_i (i = 1, 2, \cdots, 26)$ contain at least a pendant vertex, $G_1 \cong F_7(7), G_8 \cong F_8(7), G_{10} \cong F_9(7)$. By a calculation we see, for $1 \leq i \leq 26$, that

$$W(G_i, v) \leq 17 = \frac{1}{2}(7^2 - 7 - 8),$$

with equality if and only if $i = 1, 8, 10$ and v is the pendant vertex of G_1, G_8 and G_{10}, i.e., $F_7(7), F_8(7)$ and $F_9(7)$.

Assume that Eq. (4.11) holds for $n (n \geq 7)$. Let B be any graph from $B_2^1(n+1)$ with a pendant vertex v and let u be the unique neighbor of v. Then $B - v \in B_2^1(n)$, i.e., $B - v$ satisfies the induction hypothesis. So

$$W(B,v) = W(G - v, u) + n \leq \frac{1}{2}(n^2 - n - 8) + n$$

$$= \frac{1}{2}[(n+1)^2 - (n+1) - 8],$$

and equality holds if and only if u is a pendant vertex of $B - v$ and

$$B - v \in \{F_7(n), F_8(n), F_9(n)\},$$

namely $B \in \{F_7(n+1), F_8(n+1), F_9(n+1)\}$. □

Lemma 4.2. *If $n \geq 7$ and $B \in B_2^1(n)$, then we have $W(B) \leq f(n, 25, 84)$, with equality if and only if $B \in \{F_7(n), F_8(n), F_9(n)\}$.*

Proof. We prove the conclusion by induction on $n \geq 7$.

When $n = 7$, by checking $G_i (i = 1, 2, \cdots, 30)$ shown in Fig. 5, we see

$$W(G_i) \leq 42 = f(7, 25, 84),$$

with equality if and only if $i = 1, 8, 10$, i.e., $G_i \in \{F_7(7), F_8(7), F_9(7)\}$.

Suppose that the conclusion holds for $n (n \geq 7)$. Let B be any graph from $B_2^1(n+1)$. We distinguish the two following cases.

Case 1 Assume that B does not contain pendant vertices.

Now each vertex of B is contained in some cycle, i.e., B is 2-connected. For any vertex v of B, in [23] it has been proved that $W(B, v) \leq \frac{(n+1)^2}{4}$. Thus we have that

$$W(B) = \frac{1}{2} \sum_{v \in V(B)} W(B, v) \leq \frac{1}{2}(n+1) \times \frac{1}{4}(n+1)^2 < f(n+1, 25, 84).$$

Case 2 Assume that B contains at least a pendant vertex.

Let v be a pendant vertex of B and let u be the neighbor of v. Then $B - v \in B_2^1(n)$, i.e., $B - v$ satisfies the induction hypothesis. So by Lemmas 2.1 and 4.1, we get that

$$\begin{aligned} W(B) &= W(B-v) + W(B-v, u) + n \\ &\leq f(n, 25, 84) + \frac{1}{2}(n^2 - n - 8) + n = f(n+1, 25, 84), \end{aligned}$$

and equality holds if and only if u is a pendant vertex of $B - v$ and

$$B - v \in \{F_7(n), F_8(n), F_9(n)\},$$

namely $B \in \{F_7(n+1), F_8(n+1), F_9(n+1)\}$. □

It is obvious, for each graph $B \in B_2^2(n)$, that B can be obtained from B_0 by adding four rooted trees T_{x_1}, T_{y_1}, T_u, T_v with the roots x_1, y_1, u, v, respectively. In the following of this section, we always write

$$|T_{x_1}| = k+1, \quad |T_{y_1}| = l+1, \quad |T_u| = r+1, \quad |T_v| = t+1,$$

where $k + l + r + t = n - 4$. Assume, without loss of generality, that $k \geq l$ and $r \geq t$, and assume that

$$B \in B_2^2(n) - \{F_1(n), F_2(n), F_3(n), F_4(n), F_5(n), F_6(n), B_{0,0}^{n-7,3}\}. \quad (4.12)$$

Lemma 4.3. *If $n \geq 7$ and only one of k, l, r, t is not equal to* 0, *then*

$$W(B) < f(n, 25, 84).$$

Proof. Since only one of k, l, r, t is not equal to 0, from the assumptions $k \geq l$ and $r \geq t$ we see that $l = t = 0$ and only one of k and r is not equal to 0. We distinguish the two following cases.

Case 1 Assume that $k \neq 0$ and $r = 0$.

From Eq. (4.12), especially $B \ncong F_1(n)$, we see that B contains at least two pendant paths.

Subcase 1.1 Assume that B only contains two pendant paths.

At present there are integers $\delta \geq 1$, $\theta \geq 1$ and $\eta \geq 1$ with $\delta+\theta+\eta = n-3$ such that $B = B_0(x_1, \delta, \theta, \eta)$. Assume, without loss of generality, that $\theta \geq \eta$. From Eq. (4.12), especially $B \ncong F_4(n)$, it follows that $\theta \geq 2$.

If $\eta = 1$, then by Corollary 2.6 and Eq. (4.7) we have that

$$\begin{aligned} W(B) &= W(B_0(x_1, \delta, \theta, 1)) \leq W(B_0(x_1, \delta+\theta-2, 2, 1)) \\ &= W(B_0(x_1, n-6, 2, 1)) < f(n, 25, 84). \end{aligned}$$

If $\eta \geq 2$, then by Corollary 2.6 and Eq. (4.7) we have that

$$\begin{aligned} W(B) &= W(B_0(x_1, \delta, \theta, \eta)) \leq W(B_0(x_1, \delta+\theta-1, 1, \eta)) \\ &\leq W(B_0(x_1, \delta+\theta+\eta-3, 1, 2)) = W(B_0(x_1, n-6, 2, 1)) \\ &< f(n, 25, 84). \end{aligned}$$

Subcase 1.2 Assume that B contains at least three pendant paths.

In a similar way to prove Lemma 3.1, B can be transformed into a connected graph $B' \in B_2^2(n)$ containing only two pendant paths, and from the assumption of this case we know that there is a pendant path with length at least 2. Hence there exist integers $\delta \geq 1$, $\theta \geq 2$ and $\eta \geq 1$ with $\delta+\theta+\eta = n-3$ such that $B' = B_0(x_1, \delta, \theta, \eta)$. So by Corollary 2.4 and the results of Subcase 1.1 we have

$$W(B) < W(B') = W(B_0(x_1, \delta, \theta, \eta)) \leq f(n, 25, 84).$$

Case 2 Assume that $r \neq 0$ and $k = 0$.

By Eq. (4.12), especially $B \ncong F_3(n)$, we see that B has at least two pendant paths. In a similar way to prove Lemma 3.1, we can obtain a connected graph $B' \in B_2^2(n)$ that only contains two pendant paths. Thus there are integers $\delta \geq 1$, $\theta \geq 1$ and $\eta \geq 1$ with $\delta+\theta+\eta = n-3$ such that $B' = B_0(u, \delta, \theta, \eta)$. So by Corollary 2.4 we have that

$$W(B) \leq W(B') = W(B_0(u, \delta, \theta, \eta)). \tag{4.13}$$

Again by Corollary 2.6 and Eq. (4.8) we have that

$$\begin{aligned} W(B_0(u, \delta, \theta, \eta)) &\leq W(B_0(u, \delta+\theta-1, 1, \eta)) \leq W(B_0(u, \delta+\theta+\eta-2, 1, 1)) \\ &= W(B_0(u, n-5, 1, 1)) < f(n, 25, 84). \end{aligned} \tag{4.14}$$

From Eqs. (4.13) and (4.14) it follows that $W(B) < f(n, 25, 84)$. □

Lemma 4.4. *If $n \geq 7$ and at least two of k, l, r, t are not equal to 0, then*

$$W(B) < f(n, 25, 84).$$

Proof. Since at least two of k, l, r, t are not equal to 0, from the assumptions $k \geq l$, $r \geq t$ we see that $k + r \neq 0$. We distinguish the three following cases.

Case 1 Assume that $k \neq 0$ and $r \neq 0$.

Subcase 1.1 Assume that $r = 1$.

In a similar way to prove Lemma 3.1, B can be transformed into $B_{1,t}^{k,l}$. Then by applying the transformation described in Theorem 2.3, $B_{1,t}^{k,l}$ can be transformed into $B_{1,t}^{k+l,0}$. Finally by using the transformation defined in Corollary 2.5, $B_{1,t}^{k+l,0}$ can be transformed into $B_{1,0}^{k+l+t,0} = B_{1,0}^{n-5,0} = F_6(n)$. So by Corollary 2.4, Theorem 2.3, Corollary 2.5 and Eq. (4.6) we get

$$W(B) \leq W(B_{1,t}^{k,l}) \leq W(B_{1,t}^{k+l,0}) \leq W(B_{1,0}^{k+l+t,0}) = f(n, 25, 84). \quad (4.15)$$

From Eq. (4.12), especially $B \ncong F_6(n)$, we see that B contains at least three pendant vertices. This indicates that one of three transformations is performed at least once. So one inequality in Eq. (4.15) is strict. Therefore, it follows that $W(B) < f(n, 25, 84)$.

Subcase 1.2 Assume that $r \geq 2$.

In a similar way to prove Lemma 3.1, B can be transformed into $B_{r,t}^{k,l}$. Then by applying the transformation described in Theorem 2.3, $B_{r,t}^{k,l}$ can be transformed into $B_{r,t}^{k+l,0}$. Finally by using the transformation defined in Corollary 2.5, $B_{r,t}^{k+l,0}$ can be transformed into $B_{r+t,0}^{k+l,0}$.

If $k + l \geq r + t$, then by using the transformation defined in Corollary 2.5 at least once, $B_{r+t,0}^{k+l,0}$ can be transformed into $B_{1,0}^{k+l+r+t-1,0} = B_{1,0}^{n-5,0} = F_6(n)$. So by Corollary 2.4, Theorem 2.3, Corollary 2.5 and and Eq. (4.6) it follows that

$$W(B) \leq W(B_{r,t}^{k,l}) \leq W(B_{r,t}^{k+l,0}) \leq W(B_{r+t,0}^{k+l,0}) < W(F_6(n)) = f(n, 25, 84).$$

If $k+l < r+t$, then by using the transformation defined in Corollary 2.5, $B_{r+t,0}^{k+l,0}$ can be transformed into $B_{r+t+k+l-1,0}^{1,0} = B_{n-5,0}^{1,0}$. So by Corollary 2.4, Theorem 2.3, Corollary 2.5 and Eq. (4.10) it follows that

$$W(B) \leq W(B_{r,t}^{k,l}) \leq W(B_{r,t}^{k+l,0}) \leq W(B_{r+t,0}^{k+l,0}) \leq W(B_{n-5,0}^{1,0}) < f(n, 25, 84).$$

Case 2 Assume that $k = 0$ and $r \neq 0$.

At present $l = 0$ and $t \neq 0$. In a similar way to prove Lemma 3.1, B can be transformed into $B_{r,t}^{0,0}$. Again using the transformation described in Corollary 2.5, $B_{r,t}^{0,0}$ can be transformed into $B_{r+t-1,1}^{0,0} = B_{n-5,1}^{0,0}$. So by Corollaries 2.4 and 2.5 it follows that

$$W(B) \le W(B_{r,t}^{0,0}) \le W(B_{n-5,1}^{0,0}). \tag{4.16}$$

Since $W(B_{0,1}^{0,0}, x_1) = 6 > 5 = W(B_{0,1}^{0,0}, u)$ and $B_{0,1}^{n-5,0} \cong B_{1,0}^{n-5,0} = F_6(n)$, from Theorem 2.8 and Eq. (4.6) we get that

$$W(B_{n-5,1}^{0,0}) < W(B_{0,1}^{n-5,0}) = W(F_6(n)) = f(n, 25, 84). \tag{4.17}$$

By Eqs. (4.16) and (4.17) it follows that $W(B) < f(n, 25, 84)$.
Case 3 Assume that $k \neq 0$ and $r = 0$.

Now $t = 0$ and $l \neq 0$. We again distinguish the three following cases.
Subcase 3.1 Assume that $l = 1$.

By Eq. (4.12), especially $B \ncong F_2(n)$, we see that B contains at least three pendant vertices. In a similar way to prove Lemma 3.1, B can be transformed into a connected graph $B' \in \mathcal{B}_2^2(n)$ that only contains three pendant vertices. So there exist three integers $\delta \geq 1$, $\theta \geq 1$ and $\eta \geq 1$ with $\delta + \theta + \eta = n - 4$ such that $B' = B_{0,0}^{0,1}(x_1, \delta, \theta, \eta)$. By applying the transformation defined in Corollary 2.6, $B_{0,0}^{0,1}(x_1, \delta, \theta, \eta)$ can be transformed into $B_{0,0}^{0,1}(x_1, \delta + \theta + \eta - 2, 1, 1) = B_{0,0}^{0,1}(x_1, n - 6, 1, 1)$. So by Corollaries 2.4, 2.6 and Eq. (4.7) it follows that

$$W(B) \le W(B_{0,0}^{0,1}(x_1, \delta, \theta, \eta)) \le W(B_{0,0}^{0,1}(x_1, n - 6, 1, 1)) < f(n, 25, 84).$$

Subcase 3.2 Assume that $l = 2$.

At present B satisfies $deg_B(z_1) = 3$ or $deg_B(z_1) = 4$. Let M be the vertex-induced subgraph of $\{u, v, x_1, z_1\} \bigcup V(T_{z_1})$ in B.

If $deg_B(z_1) = 3$, then by Eq. (4.12), especially $B \ncong F_5(n)$, we see that B contains at least three pendant vertices. In a similar way to prove Lemma 3.1, B can be transformed into a connected graph $B' \in \mathcal{B}_2^2(n)$ that only contains three pendant vertices. So there exist integers $\delta \geq 1$, $\theta \geq 1$ and $\eta \geq 1$ with $\delta+\theta+\eta = n-5$ such that $B' = M(x_1, \delta, \theta, \eta)$. By using the transformation defined in Corollary 2.6, $M(x_1, \delta, \theta, \eta)$ can be transformed into $M(x_1, \delta + \theta + \eta - 2, 1, 1) = M(x_1, n - 7, 1, 1)$. It is easy to get that

$$W(M(x_1, n - 7, 1, 1)) = f(n, 31, 120).$$

So by Corollaries 2.4 and 2.6 we get that

$$W(B) \le W(M(x_1, \delta, \theta, \eta)) \le W(M(x_1, n - 7, 1, 1)) < f(n, 25, 84).$$

If $deg_B(z_1) = 4$, i.e., B only contains two pendant edges at z_1, then in a similar way to prove Lemma 3.1, B can be transformed into a graph

B' that is the graph obtained from M by adding a pendant path of length $n-6$ to x_1. It is easy to get that

$$W(B') = f(n, 31, 120).$$

So by Corollary 2.4 it follows that $W(B) \leq W(B') < f(n, 25, 84)$.

Subcase 3.3 Assume that $l = 3$.

Now $n \geq 10$, and by Eq. (4.12), especially $B \ncong B_{0,0}^{n-7,3}$, we see that B contains at least three pendant vertices. For $a \in \{x_1, z_1\} \subseteq V(B_0)$, let $H(a, \delta, \theta, \eta, l)$ be the n-vertex graph formed from $B_0(a, \delta, \theta, \eta)$ by adding a pendant path of length l to the vertex of $\{x_1, z_1\} - \{a\}$. Write $V_1 = V(T_{x_1}) - \{x_1\}$ and $V_2 = V(T_{z_1}) - \{z_1\}$.

Assume that V_1 contains at least two pendant vertices of B. First in a similar way to prove Lemma 3.1, B can be transformed into some graph $H(x_1, \delta, \theta, \eta, 3)$. Then by using the transformation defined in Corollary 2.6, $H(x_1, \delta, \theta, \eta, 3)$ can be transformed into $H(x_1, \delta + \theta + \eta - 2, 1, 1, 3) = H(x_1, n-8, 1, 1, 3)$. Finally by using the transformation described in Theorem 2.3 (taking $k = 2$), $H(x_1, n-8, 1, 1, 3)$ can be transformed into $H(x_1, n-6, 1, 1, 1) = B_{0,0}^{0,1}(x_1, n-6, 1, 1)$. So by Corollaries 2.4-2.6, Theorem 2.3 and Eq. (4.7) it follows that

$$\begin{aligned} W(B) &\leq W(H(x_1, \delta, \theta, \eta, 3)) \leq W(H(x_1, n-8, 1, 1, 3)) \\ &< W(H(x_1, n-6, 1, 1, 1)) = W(B_{0,0}^{0,1}(x_1, n-6, 1, 1)) \\ &\leq f(n, 25, 84). \end{aligned}$$

Assume that V_1 only contains a pendant vertex of B. Now V_2 contains at least two pendant vertices of B. First in a similar way to prove Lemma 3.1, B can be transformed into some graph $H(z_1, \delta, \theta, \eta, n-7)$. Then by using the transformation defined in Corollary 2.6, $H(z_1, \delta, \theta, \eta, n-7)$ can be transformed into $H(z_1, \delta + \theta + \eta - 2, 1, 1, n-7) = H(z_1, 2, 1, 1, n-7)$. Finally by using the transformation described in Theorem 2.3 (taking $k = n-8$), $H(z_1, 2, 1, 1, n-7)$ can be transformed into $H(z_1, n-6, 1, 1, 1) \cong B_{0,0}^{0,1}(x_1, n-6, 1, 1)$. So by Corollaries 2.4-2.6, Theorem 2.3 and Eq. (4.7) it follows that

$$\begin{aligned} W(B) &\leq W(H(z_1, \delta, \theta, \eta, n-7)) \leq W(H(z_1, 2, 1, 1, n-7)) \\ &< W(H(z_1, n-6, 1, 1, 1)) = W(B_{0,0}^{0,1}(x_1, n-6, 1, 1)) \\ &\leq f(n, 25, 84). \end{aligned}$$

Subcase 3.4 Assume that $l \geq 4$.

Now $n \geq 12$. In a similar way to prove Lemma 3.1, B can be transformed into $B_{0,0}^{k,l}$. Again by using the transformation described in Theorem 2.3, $B_{0,0}^{k,l}$ can be transformed into $B_{0,0}^{k+l-4,4} = B_{0,0}^{n-8,4}$. It is easy to see that

$$W(B_{0,0}^{n-8,4}) = f(n, 37, 222).$$

So by Corollary 2.4 and Theorem 2.3 it follows that

$$W(B) \leq W(B_{0,0}^{k,l}) \leq W(B_{0,0}^{n-8,4}) < f(n, 25, 84).$$

This proof is complete. □

On one hand, it is required that $n \geq 8$ in $F_5(n)$ and it is easy to see, by Eqs. (4.3)-(4.5), that

$$W(F_3(n)) - W(F_5(n)) = n - 8, \quad W(F_4(n)) - W(F_5(n)) = n - 9.$$

On the other hand, it is required that $n \geq 10$ in $B_{0,0}^{n-7,3}$ and it is easy to see, by Eqs. (4.6) and (4.9), that

$$W(F_5(n)) - W(B_{0,0}^{n-7,3}) = n - 9, \quad W(F_6(n)) - W(B_{0,0}^{n-7,3}) = n - 12.$$

Therefore, by Lemmas 4.2-4.4 and Eqs. (4.1)-(4.6) we get the main results in this section as follows.

Theorem 4.5. *If $n = 7$, for $B \in B_2^2(n) - \{F_i(n) : 1 \leq n \leq 9, i \neq 5\}$, then*

$$W(B) < W(F_9(n)) = W(F_8(n)) = W(F_7(n)) = W(F_6(n)) < W(F_4(n))$$
$$< W(F_3(n)) < W(F_2(n)) < W(F_1(n)).$$

If $n = 8$, for $B \in B_2^2(n) - \{F_i(n) : 1 \leq n \leq 9\}$, then

$$W(B) < W(F_9(n)) = W(F_8(n)) = W(F_7(n)) = W(F_6(n)) < W(F_4(n))$$
$$< W(F_5(n)) = W(F_3(n)) < W(F_2(n)) < W(F_1(n)).$$

If $n = 9$, for $B \in B_2^2(n) - \{F_i(n) : 1 \leq n \leq 9\}$, then

$$W(B) < W(F_9(n)) = W(F_8(n)) = W(F_7(n)) = W(F_6(n)) < W(F_5(n))$$
$$= W(F_4(n)) < W(F_3(n)) < W(F_2(n)) < W(F_1(n)).$$

If $10 \leq n \leq 12$, for $B \in B_2^2(n) - \{B_{0,0}^{n-7,3}, F_i(n) : 1 \leq n \leq 9\}$, then

$$W(B) < W(F_9(n)) = W(F_8(n)) = W(F_7(n)) = W(F_6(n)) < W(B_{0,0}^{n-7,3})$$
$$< W(F_5(n)) < W(F_4(n)) < W(F_3(n)) < W(F_2(n)) < W(F_1(n)).$$

If $n \geq 13$, for $B \in B_2^2(n) - \{F_i(n) : 1 \leq n \leq 9\}$, then

$$W(B) < W(F_9(n)) = W(F_8(n)) = W(F_7(n)) = W(F_6(n)) < W(F_5(n))$$
$$< W(F_4(n)) < W(F_3(n)) < W(F_2(n)) < W(F_1(n)).$$

5. Conclusions

Let $S_i(n)$ be the set of all n-vertex bicyclic graphs having the i-largest Wiener index. Feng et al. [17] had proved that $S_1(n) = \{F_1(n)\}$. Write

$$D_1(n) = B_1(3, n-4, 3), D_2(n) = B_1(4, n-5, 3), D_3(n) = H(3, n-5, 3, 2, 2),$$

$$D_4(n) = H(3, n-6, 3, 3, 2), D_5(n) = H(3, 1, 3, n-4, 2).$$

$$\Theta(n) = \{F_6(n), F_7(n), F_8(n), F_9(n), D_4(n), D_5(n)\}.$$

By combining Theorems 3.4, 4.5, Eqs. (3.2)-(3.5) and (4.1)-(4.6) we obtain the main results in this article as follows.

Theorem 5.1 *Assume that $n \geq 7$.*

If $n = 7$, then

$$S_2(n) = \{D_1(n)\}, \quad S_3(n) = \{F_2(n)\}, \quad S_4(n) = \{F_3(n)\},$$

$$S_5(n) = \{F_4(n), D_2(n), D_3(n)\}, \quad S_6(n) = \Theta(n).$$

If $n = 8$, then

$$S_2(n) = \{D_1(n)\}, \quad S_3(n) = \{F_2(n)\}, \quad S_4(n) = \{F_3(n), F_5(n)\},$$

$$S_5(n) = \{F_4(n), D_2(n), D_3(n)\}, \quad S_6(n) = \Theta(n).$$

If $n = 9$, then

$$S_2(n) = \{D_1(n)\}, \quad S_3(n) = \{F_2(n)\}, \quad S_4(n) = \{F_3(n)\},$$

$$S_5(n) = \{F_4(n), F_5(n), D_2(n), D_3(n)\}, \quad S_6(n) = \Theta(n).$$

If $10 \leq n \leq 12$, then

$$S_2(n) = \{D_1(n)\}, \quad S_3(n) = \{F_2(n)\}, \quad S_4(n) = \{F_3(n)\},$$

$$S_5(n) = \{F_4(n), D_2(n), D_3(n)\}, \quad S_6(n) = \{F_5(n)\},$$

$$S_7(n) = \{B_{0,0}^{n-7,3}\}, \quad S_8(n) = \Theta(n).$$

If $n \geq 13$, then

$$S_2(n) = \{D_1(n)\}, \quad S_3(n) = \{F_2(n)\}, \quad S_4(n) = \{F_3(n)\},$$

$$S_5(n) = \{F_4(n), D_2(n), D_3(n)\}, \quad S_6(n) = \{F_5(n)\}, \quad S_7(n) = \Theta(n).$$

Remark 5.2 (1) It is worth indicating that the transformations given in this paper, in especial transformations defined in Corollaries 2.4 and 2.5, are very useful. For example, since the Wiener index is strictly increasing when a non-cut edge is deleted from a graph, among all graphs given clique number c and order n, by deleting some proper edges and simply applying the transformation defined in Corollary 2.4 we can see that the unique graph with the largest Wiener index is the graph obtained by attaching a pendant path of length $n-c$ to some vertex of a clique with c vertices.

(2) There still are many problems about Wiener index not to be solved. For example, determine the graphs having the smallest or largest Wiener index among all bicyclic graphs given a matching number, characterize the graphs having the smallest or largest Wiener index among all unicyclic or bicyclic graphs given a diameter or number of pendant vertices, et al.

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