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Peripheral Wiener index of a graph

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Abstract: The *eccentricity* of a vertex v is the maximum distance between v and any other vertex. A vertex with maximum eccentricity is called a peripheral vertex. The peripheral Wiener index $PW(G)$ of a graph G is defined as the sum of the distances between all pairs of peripheral vertices of G. In this paper, we initiate the study of the peripheral Wiener index and investigate its basic properties. In particular, we determine the peripheral Wiener index of the cartesian product of two graphs and trees.

Keywords: Distance in graphs, Wiener index, peripheral Wiener index

AMS Subject classification: 05C12, 05C75

1. Introduction

Let $G = (V, E)$ be a simple connected graph with vertex set V and edge set E. The order $|V|$ of G is denoted by $n = n(G)$ and the size $|E|$ of G is denoted by $m = m(G)$. For every vertex $v \in V$, the *open neighborhood* of v is the set $N(v) = \{u \in V \mid uv \in E\}$ and the *closed neighborhood* of v is the set $N[v] = N(v) \cup \{v\}$. The *degree* of a vertex $v \in V$ is $\deg_G(v) = \deg(v) = |N(v)|$. We write K_n for the *complete* graph of order n, P_n for a *path* of order n, C_n for a cycle of order n, and $K_{m,n}$ for the complete bipartite graph with partite sets of size m and n. The *distance* $d(u, v|G)$ between the two vertices u and v of G is the length of a shortest path between u and v in G. The *eccentricity* $e_G(v)$ or $e(v)$ of a vertex v is the maximum distance between v and any other vertex u of G. The *radius* r_G or $r(G)$ of G and the *diameter* diam$G$ of G are

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the minimum and maximum eccentricity of G, respectively. A vertex with maximum eccentricity is called a peripheral vertex. The *center* $C(G)$ is the set of all vertices of minimum eccentricity and *periphery* $P(G)$ is the set of all peripheral vertices of G. That is,

$$C(G) = \{u \in V(G) | e(u) = r(G)\} \quad \text{and} \quad P(G) = \{u \in V(G) | e(u) = d(G)\}.$$

The vertices in $C(G)$ are called *central vertices.* A graph G of order n with $|C(G)| = n$ is called a *self-centered graph* and a graph G of order n with $|P(G)| = n$ is called a *peripheral* graph. *The Cartesian product* $G \times H$ of two graphs $G = (V(G), E(G))$ and $H = (V(H), E(H))$ is the graph with vertex set $V(G) \times V(H)$ where two vertices (a, x) and (b, y) are adjacent if $ab \in E(G)$ and $x = y$, or $a = b$ and $xy \in E(H)$. The hypercube Q_n is defined recursively in terms of the cartesian product of two graphs as follows: $Q_1 = K_2$ and $Q_n = Q_{n-1} \times K_2$.

The Wiener index is a graph invariant of great chemical importance and is defined as

$$W = W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v|G) \tag{1}$$

where G is the graph representation of the molecule under consideration and $d(u, v|G)$ is the distance between the vertices u and v of G. The Wiener index was introduced by Wiener in 1947 [12] for modeling the shape of organic molecules and for calculating several of their Physico-Chemical properties. This parameter has been studied by mathematician from 1979 [4] and since then this distance-based quantity has been studied extensively. For more details, we refer the reader to [2, 3], and the references therein.

Gutman, Furtula and Petrović [5] defined another distance-based graph invariant known as the terminal Wiener index of a tree as,

$$TW(T) = \sum_{1 \le i < j \le k} d(v_i, v_j|T) \tag{2}$$

where $v_1, \ldots, v_k$ are pendent vertices of T. This parameter has been studied by several authors (see for example [6, 8–10, 13]).

We note that every graph contains the peripheral vertices but may not contain a terminal vertex. Here, we introduce a new distance-based graph invariant called the *peripheral Wiener index* $PW(G)$ of a graph G. The peripheral Wiener index $PW(G)$ of a graph G is the sum of distances between all pairs of peripheral vertices of G, i.e.

$$PW(G) = \sum_{1 \le i < j \le k} d(v_i, v_j|G) \tag{3}$$

where $v_1, \ldots, v_k$ are peripheral vertices of G.

If G is the graph illustrated in Figure 1, then $P(G) = \{v_1, v_2, v_3\}$ and we have

$$\begin{aligned} PW(G) &= d(v_1, v_2|G) + d(v_1, v_3|G) + d(v_2, v_3|G) \\ &= 4 + 4 + 1 \\ &= 9. \end{aligned}$$

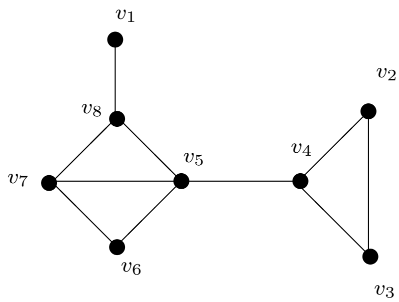

Figure 1. A graph with three peripheral vertices and peripheral Wiener index 9

The peripheral distance number of a vertex u of G, denoted by $d(u|P(G))$, is defined as

$$d(u|P(G)) = \sum_{v \in P(G)} d(u, v|G). \quad (4)$$

Clearly

$$PW(G) = \frac{1}{2} \sum_{u \in P(G)} d(u|P(G)). \quad (5)$$

For the graph illustrated in Figure 1, we have

$$\begin{aligned} d(v_1|P(G)) &= 4 + 4 = 8 \\ d(v_2|P(G)) &= 4 + 1 = 5 \\ d(v_3|P(G)) &= 4 + 1 = 5 \end{aligned}$$

and so

$$PW(G) = \frac{1}{2} \sum_{i=1}^{3} d(v_i|P(G)) = \frac{1}{2}(8 + 5 + 5) = 9.$$

In this paper, we initiate the study of the peripheral Wiener index and investigate its basic properties. In particular, we determine the peripheral Wiener index of the cartesian product of two graphs and trees.

We conclude this paper with the following observations;

Observation 1. For $n \geq 2$, $PW(K_n) = \binom{n}{2}$.

Observation 2. For $n \geq 2$, $PW(K_{1,n}) = 2\binom{n}{2}$.

Observation 3. For $n \geq m \geq 2$, $PW(K_{m,n}) = 2\binom{n}{2} + 2\binom{m}{2} + mn$.

Observation 4. Let G be a graph with exactly r peripheral vertices. Then

$$PW(G) \geq \binom{r}{2}$$

with equality if and only if $G = K_r$.

Proof. Let $v_1, \ldots, v_r$ be the peripheral vertices of G. By definition, we have

$$PW(G) = \sum_{1 \leq i < j \leq r} d(v_i, v_j|G) \geq \sum_{1 \leq i < j \leq r} 1 = \binom{r}{2}. \tag{6}$$

If $G = K_r$, then $PW(G) = \binom{r}{2}$ by Observation 1. Assume that $PW(G) = \binom{r}{2}$. We deduce from (6) that $d(v_i, v_j|G) = 1$ for each $i < j$. This implies that $\mathrm{diam}(G) = 1$ and so G is a complete graph. Since every vertex of a complete graph is a peripheral vertex, we have $G = K_r$. □

2. Relation between the peripheral Wiener index of a graph and the Wiener index of a graph

In this section, we relate the peripheral Wiener index to the Wiener index. By definition, we have $PW(G) \leq W(G)$ with equality if and only if G is a peripheral graph. Our first result is an immediate consequence of definitions.

Proposition 1. For any connected graph G, $PW(G) = W(G) = TW(G)$ if and only if $G \cong P_2$.

Next, we present a lower and an upper bound on the peripheral Wiener index of a graph G in terms of its Wiener index, order and the number of peripheral vertices.

Theorem 1. Let G be a graph of order n, diameter d and $|P(G)| = k$. Then

$$W(G) - (d-1)\left[\binom{n}{2} - \binom{k}{2}\right] \leq PW(G) \leq W(G) - \binom{n}{2} + \binom{k}{2}.$$

The equality in lower bound and upper bound holds if G is a peripheral graph.

Proof. By definition, we have

$$PW(G) = \sum_{\{u,v\} \subseteq P(G)} d(u,v|G) = W(G) - \sum_{\{u,v\} \nsubseteq P(G)} d(u,v|G).$$

Since for any $\{u,v\} \nsubseteq P(G)$ the distance $d(u,v|G)$ is at most $d-1$ and at least 1, we obtain the desired result. □

The following result is an immediate consequence of Theorem 1.

Corollary 1. Let G be a graph of order n, $\mathrm{diam}(G) = 2$ and $|P(G)| = k$. Then

$$PW(G) = W(G) - \binom{n}{2} + \binom{k}{2}.$$

Clearly, there is no graph with Wiener index two. However, in the case of the peripheral Wiener index, for any positive integer k, there exists a graph G with $PW(G) = k$. For instance, for the path $P_{k+1} := v_1 v_2 \ldots v_{k+1}$ we have $P(P_{k+1}) = \{v_1, v_{k+1}\}$ yielding

$$PW(P_{k+1}) = d(v_1, v_{k+1}|P_{k+1}) = k.$$

3. The peripheral Wiener index of a graph with diameter at most 2

In this section, we determine the peripheral Wiener index of a graph with diameter at most 2.

Theorem 2. Let G be a graph of order n, size m, diameter two and $|P(G)| = k$. Then

$$PW(G) = \binom{n}{2} + \binom{k}{2} - m.$$

Proof. Let X be the set consisting of all peripheral vertices of G and $Y = V(G) - X$. Then $|X| = k$ and $|Y| = n - k$. We conclude from $\mathrm{diam}(G) = 2$ that every vertex in Y is adjacent to all other vertices of G. Since $\sum_{u \in X} \deg(u) + \sum_{u \in Y} \deg(u) = 2m$, we deduce that

$$\sum_{u \in X} \deg(u) = 2m - (n-k)(n-1). \tag{7}$$

Since every vertex $u \in X$ is adjacent to exactly $\deg(u) - n + k$ vertices in X, we have

$$\begin{aligned} 2PW(G) &= \sum_{u \in X} (\deg(u) - n + k) + 2 \sum_{u \in X} (n - 1 - \deg(u)) \\ &= \sum_{u \in X} (n + k - 2 - \deg(u)) \\ &= kn + k^2 - 2k - 2m + (n - k)(n - 1) \text{ (by (7))} \\ &= (n^2 - n) + (k^2 - k) - 2m. \end{aligned}$$

□

The converse of Theorem 2 is not necessarily true. For example, consider the tree T in Figure 2.

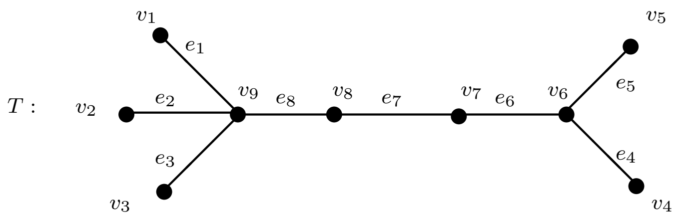

Figure 2. **A tree** T **with** $PW(T) = 38$ **and** $\text{diam}(T) \neq 2$**.**

It could be of ample interest if one could find good bounds for $PW(G)$ posed in the following open problem:

Problem 1: Let G be a graph with $\text{diam}(G) \geq 3$ and k peripheral vertices. Find upper bound for the peripheral Wiener index G.

4. Peripheral Wiener index of the Cartesian product

In this section, we study the peripheral Wiener index of the Cartesian product of graphs. The proof of the following results can be found in [7].

Lemma 1. Let G and H be connected graphs and let $(g, h), (g', h')$ be vertices of $G \times H$. Then

$$d((g, h), (g', h') | G \times H) = d(g, g' | G) + d(h, h' | H).$$

Lemma 2. Let G be the Cartesian product $\prod_{i=1}^{k} G_i$ of connected graphs and let $g = (g_1, ..., g_k)$ and $g' = (g'_1, ..., g'_k)$ be vertices of G. Then

$$d(g, g' | G) = \sum_{i=1}^{k} d(g_i, g'_i | G_i).$$

Lemma 3. For two graphs G_1 and G_2, $P(G_1 \times G_2) = P(G_1) \times P(G_2)$.

Theorem 3. Let G_i be a graph of order n_i, size m_i and with k_i peripheral vertices for $i = 1, 2$. Then

$$PW(G_1 \times G_2) = PW(G_1)\ {k_2}^2\ +\ PW(G_2)\ {k_1}^2.$$

Proof. Let $v_1, v_2, \ldots, v_{k_1}$ be the peripheral vertices of G_1 and $u_1, u_2, \ldots, u_{k_2}$ be the peripheral vertices of G_2. The peripheral Wiener indices of G_1 and G_2 are

$$PW(G_1) = \frac{1}{2} \sum_{i=1}^{k_1} \sum_{j=1}^{k_1} d(v_i, v_j | G_1) \tag{8}$$

and

$$PW(G_2) = \frac{1}{2} \sum_{k=1}^{k_2} \sum_{\ell=1}^{k_2} d(u_k, u_\ell | G_2). \tag{9}$$

By Lemma 3, we have

$$\begin{aligned}
PW(G_1 \times G_2) &= \frac{1}{2} \sum_{i=1}^{k_1} \sum_{j=1}^{k_1} \sum_{k=1}^{k_2} \sum_{\ell=1}^{k_2} d((v_i, u_k), (v_j, u_\ell) | G_1 \times G_2) \\
&= \frac{1}{2} \sum_{i=1}^{k_1} \sum_{j=1}^{k_1} \sum_{k=1}^{k_2} \sum_{\ell=1}^{k_2} \{d(v_i, v_j | G_1) + d(u_k, u_\ell | G_2)\} \quad (\textit{From Lemma 1}) \\
&= \frac{1}{2} \sum_{i=1}^{k_1} \sum_{j=1}^{k_1} \sum_{k=1}^{k_2} \sum_{\ell=1}^{k_2} d(v_i, v_j | G_1) + \frac{1}{2} \sum_{i=1}^{k_1} \sum_{j=1}^{k_1} \sum_{k=1}^{k_2} \sum_{\ell=1}^{k_2} d(u_k, u_\ell | G_2) \\
&= \frac{1}{2} \sum_{i=1}^{k_1} \sum_{j=1}^{k_1} d(v_i, v_j | G_1) \sum_{k=1}^{k_2} \sum_{\ell=1}^{k_2} 1 + \frac{1}{2} \sum_{k=1}^{k_2} \sum_{\ell=1}^{k_2} d(u_k, u_\ell | G_2) \sum_{i=1}^{k_1} \sum_{j=1}^{k_1} 1 \\
&= \frac{1}{2} \sum_{i=1}^{k_1} \sum_{j=1}^{k_1} d(v_i, v_j | G_1)(k_2 k_2) + \frac{1}{2} \sum_{k=1}^{k_2} \sum_{\ell=1}^{k_2} d(u_k, u_\ell | G_2)(k_1 k_1) \\
&= PW(G_1)\ {k_2}^2\ +\ PW(G_2)\ {k_1}^2 \quad (\textit{By } (8) \textit{ and } (9)).
\end{aligned}$$

□

Theorem 4. If G is a graph with k peripheral vertices, then

$$PW(\underbrace{G \times \cdots \times G}_{l-copies}) = l\ k^{2(l-1)}\ PW(G).$$

Proof. The proof is by induction on l. If $l = 2$, then by Theorem 3 we have

$$\begin{aligned} PW(G \times G) &= PW(G)\ k^2 \ + \ PW(G)\ k^2 \\ &= 2.k^2.PW(G) \end{aligned}$$

as desired. Let $l \geq 3$ and let the result holds for $(l-1)$, i.e

$$PW(\underbrace{G \times \cdots \times G}_{(l-1)-copies}) \ = \ (l-1)\ k^{2(l-2)}\ PW(G).$$

It follows from Theorem 3 that

$$\begin{aligned} PW(\underbrace{G \times \cdots \times G}_{(l-1)-copies}) \times G &= k^2 \ \underbrace{((l-1)\ k^{2(l-2)}\ PW(G))}_{PW(G)\ for\ (l-1)-copies} + (\underbrace{k^{l-1}}_{From\ Lemma\ 3})^2\ PW(G) \\ &= PW(G)(k^2\ (l-1)\ k^{2(l-2)} + (k^{l-1})^2) \\ &= PW(G)(k^2\ (l-1)\ k^{(2l-4)} + k^{2l-2}) \\ &= l\ PW(G)\ k^{2(l-1)}. \end{aligned}$$

This completes the proof. □

Corollary 2. If G has a unique diametral path, then

$$PW(\underbrace{G \times \cdots \times G}_{l-times}) = l.2^{2(l-1)}.\mathrm{diam}(G).$$

Proof. Let $P = v_1 \ldots v_{d+1}$ be the unique diametral path of G. Then clearly $P(G) = \{v_1, v_{d+1}\}$ and so $PW(G) = \mathrm{diam}(G)$. Now the result follows from Theorem 4. □

Corollary 3. Let Q_n $(n \geq 2)$ be the hypercube graph. Then

$$PW(Q_n) = n.2^{2(n-1)}.$$

Proof. By definition, $Q_n = \underbrace{K_2 \times \cdots \times K_2}_{n-times}$. Since $PW(K_2) = 1$, the result follows from Theorem 4. □

Since Q_n is a peripheral graph, we conclude that $PW(Q_n) = W(Q_n) = n.2^{2(n-1)}$.

5. Peripheral Wiener index of a tree

Wiener in his seminal paper [12] communicated the formula

$$W(T) = \sum_e n_1(e)n_2(e) \tag{10}$$

which holds for any tree T. In Eqn (10), e stands for an edge, whereas $n_1(e)$ and $n_2(e)$ are the number of vertices lying on two sides of e respectively and summation runs over all edges of tree T. If tree T has n vertices, then $n_1(e) + n_2(e) = n$ for all edges e. Using the same idea, Gutman et al. [5], obtained the following formula to compute the terminal Wiener index of a tree T of order n with k terminal vertices (pendent vertices):

$$TW(T) = \sum_e p_1(e)p_2(e) \tag{11}$$

where $p_1(e)$ and $p_2(e)$ are the number of terminal vertices lying on two sides of e respectively and the summation is taken over all the $(n-1)$ edges of T.
Following the above idea, we have made an attempt to calculate the peripheral Wiener index of a n-vertex tree T with k peripheral vertices.

Theorem 5. Let T be a tree of order n with k peripheral vertices. Then

$$PW(T) = \sum_{e \in E(T)} a_1(e)a_2(e) \tag{12}$$

where $a_1(e)$ and $a_2(e)$ are the number of peripheral vertices of T lying on the two sides of e.

Proof. Instead of summing distances between all pairs of peripheral vertices in a n-vertex tree T, one can pick a particular edge e which lies on a peripheral path and count how many times this edge e lies on a peripheral path, then add these counts over all edges of the underlying tree, starting from an edge e. If $a_1(e)$ is the number of peripheral vertices lying on one side of e, then $k - a_1(e)$ are the peripheral vertices lying on the other side of e. Thus, their number is $a_1(e)(k - a_1(e))$, which gives Eqn (12). □

Now one can observe that for all edges of the tree T, $a_1(e)+a_2(e) = k$ and $a_1(e)a_2(e) \geq 0$. As one can check in Figure 3, for the edges e_5 and e_6 we have $a_1(e_5) = 4$ and $a_2(e_5) = k - a_1(e_5) = 0$ while $a_1(e_6) = 4$ and $a_2(e_6) = k - a_1(e_6) = 0$. Thus, $k = 4$.

Theorem 6. Let T be a tree of order $n \geq 2$ with $|P(T)| = k$ and diameter d. Then

$$k\left(\frac{d + 2k - 4}{2}\right) \leq PW(T) \leq d\left(\frac{k(k-1)}{2}\right).$$

Furthermore, the equality holds in upper bound if every pair of peripheral vertices is at distance d and it holds in lower bound if and only if $k = 2$ or $d = 2$.

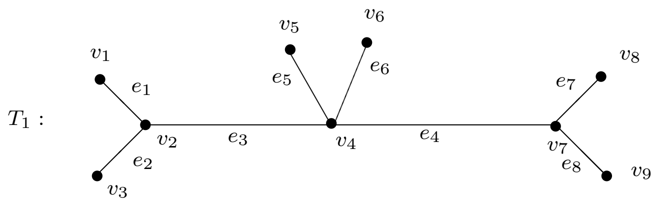

Figure 3. **A tree with peripheral Wiener index** 20

Proof. Let $u_1, \ldots, u_k$ be the peripheral vertices of T. Since T is tree, we conclude that $\deg(u_1) = \cdots = \deg(u_k) = 1$. First, we prove the lower bound. By (5), we have

$$\begin{aligned} PW(T) &= \frac{1}{2}\sum_{i=1}^{k} d(u_i|P(T)) \\ &= \frac{1}{2}(d(u_1|P(T)) + d(u_2|P(T)) + \cdots + d(u_k|P(T))) \\ &\geq \frac{1}{2}((d+2+\cdots+2) + (d+2+\cdots+2) + \cdots + (d+2+\cdots+2)) \\ &= \frac{k}{2}(d + \underbrace{2+2+\cdots+2}_{k-2}) \\ &= k(\frac{d+2k-4}{2}). \end{aligned}$$

If $k = 2$, then clearly $PW(T) = d = k(\frac{d+2k-4}{2})$. If $d = 2$, then T is a star and the result follows by Observation 2.
Conversely, let $PW(T) = k(\frac{d+2k-4}{2})$. If $k = 2$, then we are done. Assume that $k \geq 3$. Then we must have $d(u_i|P(T)) = d + 2 + \cdots + 2$ for each $i = 1, \ldots, k$. We claim that all peripheral vertices have a common neighbor. Assume without loss of generality that $d(u_1, u_2|T) = d$ and let $u_1w_1 \ldots w_{d-1}u_2$ be a diametral path in T. Then $d(u_1, u_i|T) = d(u_2, u_i|T) = 2$ for each $3 \leq i \leq k$. Since $d(u_1, u_i|T) = d(u_2, u_i|T) = 2$, u_i has a common neighbor with u_1 and u_2. It follows from $\deg(u_1) = \deg(u_2) = 1$ that $w_1 \in N(u_1) \cap N(u_i)$ and $w_{d-1} \in N(u_2) \cap N(u_i)$ for $i = 3, \ldots, k$. Since $\deg(u_3) = \cdots = \deg(u_k) = 1$, we must have $w_1 = w_{d-1}$. Thus $d = 2$, as desired.
Now we prove the upper bound. Since the distance between every two peripheral vertices is at most d, we obtain

$$PW(T) = \sum_{\{u,v\}\subseteq P(G)} d(u, v|G) \tag{13}$$

$$\leq d \sum_{\{u,v\}\subseteq P(G)} 1$$

$$\leq d(\frac{k(k-1)}{2}). \tag{14}$$

Clearly, the equality holds (14) if every pair of peripheral vertices are at distance d. □

Now, we determine the peripheral Wiener index of trees with diameter at most four. If $\mathrm{diam}(T) = 1$, then $T = K_2$. Hence $PW(T) = 1$. If $\mathrm{diam}(T) = 2$, then T is a star and so $PW(T) = 2\binom{|V(T)|-1}{2} = (|V(T)| - 1)(|V(T)| - 2)$. If $\mathrm{diam}(T) = 3$, then T is a double star $S_{m,n}$ and hence $PW(T) = 3mn + 2m + 2n$.

Proposition 2. Let T be a tree of order n with diameter 4. Let u be the central vertex of T, $N(u) = \{v_1, \dots, v_s\}$ and $A_i = N(v_i) - \{u\}$ for $i = 1, 2, \dots, s$. Then

$$PW(T) = 4 \sum_{1 \le i < j \le s} |A_i||A_j| + \sum_{i=1}^{s} |A_i|(|A_i| - 1). \tag{15}$$

Proof. Since $\mathrm{diam}(T) = 4$, T is a unicentral tree. Let $Y = \{v \in V(T) |\ d(u, v) = 2\}$.

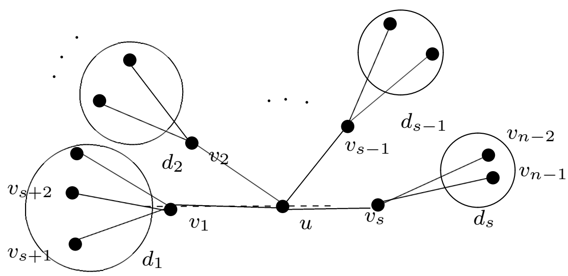

Figure 4. **A tree of order n and diameter 4**

Then, $N[u] \cup Y = V(T)$ and $Y = \cup_{i=1}^{s} A_i = P(G)$. By definition, we have

$$\begin{aligned} PW(T) &= \sum_{\{x,y\} \subseteq P(G)} d(x, y|G) \\ &= \sum_{i=1}^{s} \sum_{\{x,y\} \subseteq A_i} d(x, y|G) + \sum_{1 \le i < j \le s} \sum_{x \in A_i \& y \in A_j} d(x, y|G) \\ &= \sum_{i=1}^{s} \sum_{\{x,y\} \subseteq A_i} 2 + \sum_{1 \le i < j \le s} \sum_{x \in A_i \& y \in A_j} 4 \\ &= \sum_{i=1}^{s} |A_i|(|A_i| - 1) + 4 \sum_{1 \le i < j \le s} |A_i||A_j|, \end{aligned}$$

as desired. □

Theorem 7. Let T be a tree of order n and let $\overline{T}$ be the connected complement of T. Then

(a) $PW(\overline{T}) = 3$ if and only if $\mathrm{diam}(T) = 3$.

(b) $PW(\overline{T}) = \frac{n^2+n-2}{2}$ if and only if $\mathrm{diam}(T) > 3$.

Proof. (a) Assume that $\mathrm{diam}(T) = 3$. Then $T \cong S_{n_1,n_2}$ is a double star on n_1+n_2+2 vertices with exactly n_1+n_2 peripheral vertices. Let u and v be two central vertices of S_{n_1,n_2}. Then u and v are the peripheral vertices of $\overline{T}$ and remaining n_1+n_2 vertices of T are non-peripheral vertices of $\overline{T}$. Since $d(u,v|\overline{T}) = 3$, we have $PW(\overline{T}) = 3$.
Conversely, let $PW(\overline{T}) = 3$. Suppose, to the contrary, that $\mathrm{diam}(T) \neq 3$. Then either $\mathrm{diam}(T) \leq 2$ or $\mathrm{diam}(T) \geq 4$. If $\mathrm{diam}(T) \leq 2$, then $\overline{T}$ is disconnected, which is a contradiction. Hence $\mathrm{diam}(T) \geq 4$. Then $\mathrm{diam}(\overline{T}) \leq 2$ (see [1, 11]). Since T is connected, we must have $e_{\overline{T}}(v) = 2$ for each $v \in V(\overline{T})$. Thus, $\overline{T}$ is a self-centered graph of diameter 2. It follows from Theorem 2 that

$$PW(\overline{T}) = \binom{n}{2} + \binom{k}{2} - m = 2\binom{n}{2} - \binom{n-1}{2} = \frac{n^2+n-2}{2}. \tag{16}$$

By assumption, we must have $3 = \frac{n^2+n-2}{2}$ yielding $n = \frac{-1\pm\sqrt{33}}{2}$ which is impossible. Therefore, $\mathrm{diam}(T) = 3$.
(b) Let $\mathrm{diam}(T) \geq 4$. Using the above argument, we obtain $e_{\overline{T}}(v) = 2$ for each vertex $v \in V(T)$, and as above, we have $PW(\overline{T}) = \frac{n^2+n-2}{2}$.
Conversely, let $PW(\overline{T}) = \frac{n^2+n-2}{2}$. Since $\overline{T}$ is connected, we have $\mathrm{diam}(T) \geq 3$. If $\mathrm{diam}(T) = 3$, then by (a) we must have $3 = \frac{n^2+n-2}{2}$ that leads to a contradiction. Thus $\mathrm{diam}(T) \geq 4$ and the proof is complete. □

In the sequel, we determine the peripheral Wiener Index of two classes of trees including caterpillars. A *caterpillar* is a tree such that removal of all its leaves produces a path, called its *spine*. The *code* of the caterpillar having spine $P_s = (v_1, \ldots, v_s)$ is the ordered s-tuple $(\ell_1, \ldots, \ell_s)$, where ℓ_i is the number of leaves adjacent to v_i. Let T be a caterpillar with spine $P_s = (v_1, \ldots, v_s)$ and code $(\ell_1, \ldots, \ell_s)$. Suppose $u_1, \ldots, u_{\ell_1}$ are the leaves adjacent to v_1 and $w_1, \ldots, w_{\ell_s}$ are the leaves adjacent to v_s. Then clearly $P(T) = \{u_1, \ldots, u_{\ell_1}, w_1, \ldots, w_{\ell_s}\}$ and by definition we have

$$\begin{aligned} PW(T) &= \sum_{1\leq i<j\leq \ell_1} d(u_i,u_j|T) + \sum_{1\leq r<k\leq \ell_s} d(w_r,w_k|T) + \sum_{1\leq i\leq \ell_1, 1\leq ri\leq \ell_s} d(u_i,w_r|T) \\ &= 2\binom{\ell_1}{2} + 2\binom{\ell_s}{2} + \ell_1\ell_s(s+1) \\ &= \ell_1(\ell_1-1) + \ell_s(\ell_s-1) + \ell_1\ell_s(s+1). \end{aligned}$$

Let T_1 be a tree obtained from a caterpillar T with spine $P_s = (v_1, \ldots, v_s)$ and code $(\ell_1, 0, \ell_3, \ldots, \ell_s)$ by adding a star $K_{1,\ell}$ and joining its center to v_2. Suppose $u_1, \ldots, u_{\ell_1}$ are the leaves adjacent to v_1, $w_1, \ldots, w_{\ell_s}$ are the leaves adjacent to v_s, and $z_1, \ldots, z_\ell$ are the leaves of added star. Then $P(T) = \{u_1, \ldots, u_{\ell_1}, w_1, \ldots, w_{\ell_s}, z_1, \ldots, z_\ell\}$. By definition we have

$$\begin{aligned} PW(T) &= \sum_{1\le i<j\le \ell_1} d(u_i, u_j|T) + \sum_{1\le r<k\le \ell_s} d(w_r, w_k|T) + \sum_{1\le m<t\le \ell} d(z_m, z_t|T) + \\ &\quad \sum_{1\le i\le \ell_1 \text{ and } 1\le r\le \ell_s} d(u_i, w_r|T) + \sum_{1\le i\le \ell_1 \text{ and } 1\le m\le \ell} d(u_i, z_m|T) + \\ &\quad \sum_{1\le r\le \ell_s \text{ and } 1\le m\le \ell} d(w_r, z_m|T) \\ &= 2\binom{\ell_1}{2} + 2\binom{\ell_s}{2} + 2\binom{\ell}{2} + (\ell+\ell_1)\ell_s(s+1) + 4\ell\ell_1 \\ &= \ell_1(\ell_1-1) + \ell_s(\ell_s-1) + \ell(\ell-1) + (\ell+\ell_1)\ell_s(s+1) + 4\ell\ell_1. \end{aligned} \tag{17}$$

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