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THE MULTIPLICATIVE VERSION OF WIENER INDEX†

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Abstract. The multiplicative version of Wiener index (π-index), proposed by Gutman et al. in 2000, is equal to the product of the distances between all pairs of vertices of a (molecular) graph G. In this paper, we first present some sharp bounds in terms of the order and other graph parameters including the diameter, degree sequence, Zagreb indices, Zagreb coindices, eccentric connectivity index and Merrifield-Simmons index for π-index of general connected graphs and trees, as well as a Nordhaus-Gaddum-type bound for π-index of connected triangle-free graphs. Then we study the behavior of π-index upon the case when removing a vertex or an edge from the underlying graph. Finally, we investigate the extremal properties of π-index within the set of trees and unicyclic graphs.

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1. Introduction

As one of its main research directions, chemical graph theory [28] designs and applies the so-called molecular topological indices – numerical structure descriptors that can be calculated from the molecular graph [28, 13]. Among numerous topological indices put forward in the chemical literature, only a few found noteworthy chemical and/or physio-chemical applications. The first such a molecular topological index was the Wiener index, put forward by Wiener [31] in 1947. Although it was invented a long time ago, Wiener index is still extensively used in quantitative structure-property and structure-activity studies. The *Wiener index* of a graph G, denoted by $W(G)$, is defied as

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

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Wiener index gained much popularity during the past several decades, and its many mathematical properties have been explored, see [6, 8, 9, 16, 23, 25, 27, 29, 30] and the references cited therein.

In [11, 12], the *multiplicative version of the Wiener index* was conceived by Gutman et al.:

$$\pi = \pi(G) = \prod_{\{u,\, v\} \subseteq V(G)} d_G(u,\, v). \tag{1}$$

It can be seen from Eq. (1) that adjacent vertex pairs in an underlying graph play no role in contributing to the π-index. That is, the π-index reflects only long-distance structural features of a molecule. From this, we may conclude that the properties of π and W are different to some extent. In [11, 12] Gutman et al. showed that in the case of alkanes there exists a very good correlation between π and W, and there exists a (either linear or slightly curvilinear) correlation between π and W among a variety of classes of isomeric alkanes, monocycloalkanes, bicycloalkanes, benzenoid hydrocarbons, and phenylenes. Aparting from the above two chemical literatures, there exists no other existing literatures studying the π-index, especially for its mathematical properties.

From the viewpoint of graph theory, we are concerned with the properties of a new graph parameter. Concerning the extremal properties of π-index, it has been proved that [11] among all nontrivial trees, the star is the unique graph with the minimum π-index and the path is the unique graph with the maximum π-index. Moreover, Gutman et al. [11] proved that among all nontrivial connected graphs, the path is the unique graph with the maximum π-index, while the complete graph is the unique graph with the minimum π-index. Since then, there exist no results dealing with further mathematical properties of π-index in the existing literatures.

In this paper, we aim at exploring further properties of π-index. This paper is organized as follows. In Section 1, we present some sharp bounds in terms of the order and other graph parameters including the diameter, degree sequence, Zagreb indices, Zagreb coindices, eccentric connectivity index and Merrifield-Simmons index for π-index of general connected graphs and trees, as well as a Nordhaus-Gaddum-type bound for π-index of connected triangle-free graphs. In Section 2, we study the behavior of π-index upon the case when removing a vertex or an edge from the underlying graph. In the last section, we investigate the extremal properties of π-index within the set of trees and unicyclic graphs.

Before proceeding, we introduce some notation and terminology. For a graph G, let $d_G(v)$ be the degree of a vertex v in G. Let $\delta(G)$ and $\triangle(G)$ denote the minimum and maximum vertex degree in a graph G, respectively. The distance between two vertices u and v in a graph G is denoted by $d_G(u,\, v)$. The *eccentricity* of a vertex v in a connected graph G is defined as $ec_G(v) = \max\{d_G(v,\, u) | u \in V(G)\}$. A *tree* is a connected graph having no cycles. A *unicyclic graph* is a connected graph whose number of vertices equals to number of edges. Other notation and terminology not defined here, the reader is referred to [3].

2. Sharp bounds on π-index involving other graph parameters

In this section, we shall give some sharp bounds for π-index of connected graphs including other graph parameters such as the order, diameter, degree sequence and Merrifield-Simmons index. Moreover, we provide several sharp lower bounds for π-index of trees in terms of other graph invariants including the eccentric connectivity index, Zagreb indices and Zagreb coindices. Furthermore, we present a Nordhaus-Gaddum-type lower bound for π-index of connected triangle-free graphs.

Let $D(G,k)$ denote the number of vertex pairs in G that are at distance k. Clearly, $\sum_{k\geq 1} D(G,k) = \binom{n}{2} = \frac{n(n-1)}{2}$. Thus, we can rewrite Eq. (1) as

$$\pi(G) = \prod_{k\geq 1} k^{D(G,\,k)}. \tag{2}$$

The following result is immediate by using Eq. (2).

Theorem 1. *Let G be a connected graph of order n and diameter d. Then*

$$1 \leq \pi(G) \leq d^{\binom{n}{2}},$$

with either equality if and only if $d = 1$, that is, $G \cong K_n$.

In the following, we shall give an upper bound for the multiplicative Wiener index of connected graphs in terms of its order and degree sequence. We first summarize here a result of [21] as the following lemma.

Lemma 1. *Let G be a nontrivial connected graph of order n. For each vertex v in G, it holds*

$$ec_G(v) \leq n - d_G(v).$$

Moreover, all equalities hold together if and only if $G \cong P_4$ or $K_n - iK_2$ $(0 \leq i \leq \lfloor \frac{n}{2} \rfloor)$, where $K_n - iK_2$ denotes the graph obtained by removing i independent edges from G.

Theorem 2. *Let G be a nontrivial connected graph of order n and degree sequence $(d_1, d_2, \ldots, d_n)$. Then*

$$\pi(G) \leq \sqrt{\prod_{i=1}^{n} (n-d_i)^{n-d_i-1}}$$

with equality if and only if $G \cong P_4$ or $K_n - iK_2$ $(0 \leq i \leq \lfloor \frac{n}{2} \rfloor)$.

Proof. For any given vertex v in G, we write $\widetilde{D}_G(v) = \prod_{u\in V(G)\setminus\{v\}} d_G(u,\, v)$.

Then

$$\pi(G) = \prod_{k\geq 1} k^{D(G,\,k)} = \sqrt{\prod_{v\in V(G)} \widetilde{D}_G(v)}.$$

For consistence, if $d_G(v) = n-1$, then we set $\prod_{u\in V(G)\setminus N_G[v]} d_G(u,\,v) = 1$. By this definition, we have $\widetilde{D}_G(v) = \prod_{u\in V(G)\setminus N_G[v]} d_G(u,\,v)$ for any vertex $v\in V(G)$.

By Lemma 1,

$$\begin{aligned}\widetilde{D}_G(v) &= \prod_{u\in V(G)\setminus N_G[v]} d_G(u,\,v)\\ &\leq \prod_{u\in V(G)\setminus N_G[v]} ec_G(v)\\ &\leq \prod_{u\in V(G)\setminus N_G[v]} (n-d_G(v))\\ &= (n-d_G(v))^{n-d_G(v)-1}.\end{aligned}$$

The above first equality holds if and only if $d_G(u,\,v) = ec_G(v)$ for any $u\in V(G)\setminus N_G[v]$, that is, $ec_G(v)\leq 2$. The above second equality holds if and only if $ec_G(v) = n-d_G(v)$.

Hence, by Lemma 1,

$$\begin{aligned}\pi(G) &= \sqrt{\prod_{v\in V(G)} \widetilde{D}_G(v)}\\ &\leq \sqrt{\prod_{v\in V(G)} (n-d_G(v))^{n-d_G(v)-1}}\\ &= \sqrt{\prod_{i=1}^{n}(n-d_i)^{n-d_i-1}}\end{aligned}$$

with equality holds if and only if $G\cong P_4$ or $K_n - iK_2$ $(0\leq i\leq \lfloor \frac{n}{2}\rfloor)$. □

From Theorem 2 it follows readily the following consequence.

Corollary 2.1. *Let G be a nontrivial connected graph of order n and minimum degree δ. Then*

$$\pi(G)\leq (n-\delta)^{\frac{n(n-\delta-1)}{2}}$$

with equality if and only if $G\cong K_n$ or or an $(n-2)$-regular graph.

A vertex subset S of a graph G is said to be an *independent set* of G, if the subgraph induced by S is an empty graph. Then

$$\beta = \max\{|S| : S \text{ is an independent set of } G\}$$

is said to be the *independence number* of G.

The *Merrifield-Simmons index* of a graph G (see [17, 18]) is defined as

$$i(G) = \sum_{k \geq 0} i(G; k),$$

where $i(G; k)$ is the number of k-membered independent sets in G for $k \geq 1$, and it is usually assumed that $i(G; 0) = 1$ for the sake of convenience and consistence.

In the following result, we shall present a sharp upper bound for π-index in terms of the order, diameter and Merrifield-Simmons index of the underlying graph.

Theorem 3. *Let G be a nontrivial connected graph of order n and diameter $d \geq 2$. Then*

$$\pi(G) \leq d^{i(G)-n-1}$$

where the equality is attained if and only if $d = 2$ and the independence number of G is exactly two.

Proof. It is obvious that the number of vertex pairs $\{u, v\}$ in G at distance greater than or equal to two is exactly $i(G; 2)$. Moreover, we have

$$i(G) \geq 1 + n + i(G; 2)$$

with equality if and only if the independence number of G is equal to 2. That is,

$$i(G; 2) \leq i(G) - n - 1$$

with equality if and only if the independence number of G is equal to 2.

Then

$$\begin{aligned} \pi(G) &= \prod_{k \geq 1} k^{D(G,k)} \\ &\leq d^{\sum_{k \geq 2} D(G,k)} \\ &= d^{i(G;2)} \\ &\leq d^{i(G)-n-1}. \end{aligned}$$

The equality is attained in the above first inequality if and only if $d = 2$, and the equality is attained in the above second inequality if and only if the independence number of G is exactly two. This proves theorem. □

Remark 1. Consider the sharpness of bound in Theorem 3. It is easy to see that $K_n - iK_2\, (1 \leq i \leq \lfloor \frac{n}{2} \rfloor)$ and the cycle C_5 attain the bound.

In the following, we shall give sharp lower bounds for π-index of the underlying trees in terms of the Zagreb indices, the first Zagreb coindex, or the eccentricity index.

Let $M_1(G) = \sum_{v \in V(G)} (d_G(v))^2$ and $M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v)$ denote, respectively, the first and second Zagreb index of a graph G (see [4, 15, 22, 24, 33, 34]). It is obvious that one can rewrite the first Zagreb index as $M_1(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v))$.

Theorem 4. *Let T be a tree with n vertices and diameter at least three. Then*

$$\pi(T) \geq \left(\frac{3}{2}\right)^{n-1} \cdot 3^{M_2(T)} \cdot \left(\frac{\sqrt{2}}{3}\right)^{M_1(T)}$$

with equality if and only if T is a double star.

Proof. Let $\#P_k(T)$ denote the number of k-vertex paths in T. Then $\#P_1(T) = n$, $\#P_2(T) = n-1$. Moreover, $\#P_3(T) = \sum_{v \in V(T)} \binom{d_T(v)}{2} = \sum_{v \in V(T)} \frac{d_T(v)(d_T(v)-1)}{2} = \frac{1}{2}M_1(T) - n + 1$ and $\#P_4(T) = \sum_{uv \in E(T)} (d_T(u)-1)(d_T(v)-1) = M_2(T) - M_1(T) + n - 1$.

By Eq. (2),

$$\pi(T) \geq 2^{\#P_3(T)} 3^{\#P_4(T)}$$

with equality if and only if $d = 3$.

That is,

$$\begin{aligned}\pi(T) &\geq 2^{\frac{1}{2}M_1(T) - n + 1} 3^{M_2(T) - M_1(T) + n - 1} \\ &= \left(\frac{3}{2}\right)^{n-1} \cdot 3^{M_2(T)} \cdot \left(\frac{\sqrt{2}}{3}\right)^{M_1(T)}\end{aligned}$$

with equality if and only if T is a double star.

This completes the proof. □

For a nontrivial graph G, let $\overline{M}_1(G) = \sum_{uv \notin E(G)} (d_G(u) + d_G(v))$ denote *the first Zagreb coindex* (see [1, 2, 14, 19]). It is obvious that one can rewrite $\overline{M}_1(G) = \sum_{u \in V(G)} d_G(u)(n - d_G(u) - 1) = 2m(n-1) - M_1(G)$, where n and m are, respectively, the number of number of vertices and edges in G. Using this fact and Theorem 4, we get the following result.

Corollary 2.2. *Let T be a tree with n vertices and diameter at least three. Then*

$$\pi(T) \geq \left(\frac{3}{2}\right)^{n-1} \cdot 3^{M_2(T)} \cdot \left(\frac{\sqrt{2}}{3}\right)^{2n(n-1) - \xi^c(T)}$$

with equality if and only if $T \cong P_4$.

For a nontrivial graph G, let $\xi^c(G) = \sum_{u \in E(G)} ec_G(u) d_G(u)$ denote *the eccentric connectivity index* (see [5, 7, 20, 35]).

Corollary 2.3. *Let T be a tree with n vertices and diameter at least three. Then*

$$\pi(T) \geq \left(\frac{3}{2}\right)^{n-1} \cdot 3^{M_2(T)} \cdot \left(\frac{\sqrt{2}}{3}\right)^{2n(n-1)-\xi^c(T)}$$

with equality if and only if $T \cong P_4$.

Proof. According to Lemma 1, we have

$$\begin{aligned}\xi^c(T) &= \sum_{v \in V(G)} ec_T(v) d_T(v) \\ &\leq \sum_{v \in V(T)} (n - d_T(v)) d_T(v) \\ &= 2mn - M_1(T),\end{aligned}$$

with equality if and only if $ec_T(v) = n - d_T(v)$ holds for each vertex v in T, that is, $T \cong P_4$.

Hence, $M_1(T) \leq 2mn - \xi^c(T) = 2n(n-1) - \xi^c(T)$ with the equality if and only if $T \cong P_4$.

Note that $\left(\frac{\sqrt{2}}{3}\right)^x$ is an decreasing function. Then $\left(\frac{\sqrt{2}}{3}\right)^{M_1(T)} \geq \left(\frac{\sqrt{2}}{3}\right)^{2n(n-1)-\xi^c(T)}$ with equality if and only if $T \cong P_4$.

Combining this fact and Theorem 4, we obtain

$$\pi(T) \geq \left(\frac{3}{2}\right)^{n-1} \cdot 3^{M_2(T)} \cdot \left(\frac{\sqrt{2}}{3}\right)^{2n(n-1)-\xi^c(T)}$$

with equality if and only if $T \cong P_4$. This completes the proof. □

In the following, we give a Nordhaus-Gaddum-type result for the π-index of connected triangle-free graphs. Suppose that G is a connected triangle-free graph on n vertices such that $\overline{G}$ is connected. Then we clearly have $n \geq 4$. If $n = 4$, then G must be isomorphic to the path P_4. So we will assume that $n \geq 5$ in our following theorem.

Theorem 5. *Let G be a connected triangle-free graph of order $n \geq 5$ and $\overline{G}$ be its connected complement. Then*

$$\ln \pi(G) + \ln \pi(\overline{G}) \geq \binom{n}{2} \ln 2,$$

with equality if and only if $G \cong C_5$ or $\overline{G} \cong C_5$.

Proof. Let d and $\overline{d}$ denote the diameters of G and $\overline{G}$, respectively. By the definition,

$$\ln \pi(G) \geq \left[\binom{n}{2} - m\right] \ln 2$$

with the equality if and only if $d = 2$.

Let m and $\overline{m}$ denote the number of edges in G and $\overline{G}$, respectively. Similar to above,

$$\ln \pi(\overline{G}) \geq \left[\binom{n}{2} - \overline{m}\right] \ln 2$$

with the equality if and only if $\overline{d} = 2$.

Note that $m + \overline{m} = \binom{n}{2}$. According to the above two inequalities,

$$\ln \pi(G) + \ln \pi(\overline{G}) \geq \binom{n}{2} \ln 2,$$

with the equality if and only if $d = 2$ and $\overline{d} = 2$.

Assume first that $\ln \pi(G) + \ln \pi(\overline{G}) = \binom{n}{2} \ln 2$. Then $d = 2$ and $\overline{d} = 2$. We claim that G has no pendent vertices. Suppose to the contrary that there exists a pendent vertex v in G and let u be its unique neighbor. Since $d = 2$, we must have $d_G(u) = n - 1$. But then $\overline{G}$ is disconnected. Hence $\delta(G) \geq 2$.

If $\triangle(G) = 2$, then G is just a cycle C_n. Since $d = 2$ and $\overline{d} = 2$, we thus have $n = 5$, that is, $G \cong C_5$ ($\overline{C_4}$ is disconnected).

Assume now that $\triangle(G) \geq 3$. Let v be a vertex in G with $d_G(v) = \triangle$ and let $N_G(v) = \{v_1, v_2, \ldots, v_\triangle\}$. Since G is triangle-free, then $G[v_1, v_2, \ldots, v_\triangle]$ is a null graph. Thus, for any vertex u in $V(G) \setminus N_G[v]$, we have $uv_i \in E(G)\,(i = 1, \ldots, \triangle)$, since $d = 2$. Let $A = N_G(v) = \{v_1, v_2, \ldots, v_\triangle\}$ and $B = V(G) \setminus A$. If there exist two vertices, say x and y, in $B \setminus \{v\}$ such that $xy \in E(G)$, then G contains triangles $v_i x y v_i\,(i = 1, \ldots, \triangle)$, a contradiction. Thus, G is the complete bipartite graph $K_{\triangle,\, n-\triangle}$ with one partite set being A and another partite set being B. But then, $\overline{G} = \overline{K_{\triangle,\, n-\triangle}}$ is disconnected, a contradiction to our assumption. The arguments above lead us to that $\ln \pi(G) + \ln \pi(\overline{G}) = \binom{n}{2} \ln 2$ only if $G \cong C_5$.

Conversely, we have $\ln \pi(C_5) + \ln \pi(\overline{C_5}) = 10 \ln 2 = \binom{n}{2} \ln 2$. This completes the proof. □

3. The effect of the removal of a vertex or an edge on π-index

In this section, we study the behavior of π-index upon the case when a vertex or an edge is removed from the underlying graph. More precisely, we prove the following two results.

Proposition 1. *Let G be a nontrivial n-vertex connected graph.*

(i) If $e = uv$ is not a cut edge in G, then $\pi(G - e) \geq 2\pi(G)$;

(ii) If w is not a cut vertex in G and $d_G(w) = n - 1$, then $\pi(G - w) \geq \pi(G)$.

Proof. For (i), one can easily see that $d_{G-e}(x, y) \geq d_G(x, y)$ for any two vertices x and y in G. Moreover, $d_{G-e}(u, v) \geq 2 = 2d_G(u, v)$. Hence, $\pi(G - e) \geq 2\pi(G)$, as desired.

Let us proceed to (ii). Let $\widetilde{D}_G(v)$ be the same quantity as defined in Theorem 2. Since $d_G(w) = n-1$, we have

$$\pi(G) = \sqrt{\prod_{v\in V(G)} \widetilde{D}_G(v)} = \sqrt{\prod_{v\in V(G)\setminus\{w\}} \widetilde{D}_G(v)}$$
$$\leq \sqrt{\prod_{v\in V(G)\setminus\{w\}} \widetilde{D}_{G-w}(v)} = \pi(G-w),$$

as claimed. □

Remark 2. The equality in (i) can be attained at the graph C_3 or the graph S_n^+. The equality in (ii) can also be attained at many graph families. For instance, both the complete graph K_n and the graph $K^*_{2,\,n-2}$, obtained from the complete graph $K_{2,\,n-2}$ by adding an edge between two vertices of degree $n-2$, achieve this equality.

4. Extremal trees and unicyclic graphs w.r.t. the π-index

In this section, we characterize the n-vertex tree and unicyclic graph with the maximum π-index. To do this, we need to introduce two kinds of graph transformations on π-index as introduced in the following lemma.

Lemma 2. *Let w be a vertex of a nontrivial connected graph G. For nonnegative integers p and q, let $G(s,t)$ denote the graph obtained from G by attaching to vertex w pendant paths $P = wv_1v_2\dots v_s$ and $Q = wu_1u_2\dots u_t$ of lengths s and t, respectively. Let $G(s+t,0) = G(s,t) - wu_1 + v_su_1$.*
(i). If $s \geq t \geq 1$, then $\pi(G(s+t,0)) > \pi(G(s,t))$;
(ii). If $s \geq t \geq 2$, then $\pi(G(s+1,t-1)) > \pi(G(s,t))$.

Proof. We only prove (i) here. The proof of (ii) can be conducted by the same way. For any two vertices x, y in $V(G)$, $d_{G(s+t,0)}(x,\,y) = d_{G(s,t)}(x,\,y)$. Similarly, for any vertex x in $V(G)$ and v_i, $i = 1,\,\dots,\,s$, $d_{G(s+t,0)}(x,\,v_i) = d_{G(s,t)}(x,\,v_i)$. Moreover, for any pair of vertices x, y in $\{v_1,\,\dots,\,v_s; u_1,\,\dots,\,u_t\}$ of $G(s,t)$, there exists a pair of vertices x', y' in $\{v_1,\,\dots,\,v_s; u_1,\,\dots,\,u_t\}$ of $G(s+t,0)$ such that $d_{G(s+t,0)}(x',\,y') = d_{G(s,t)}(x,\,y)$. However, for each vertex x in $V(G)$ and each u_j, $j = 1,\,\dots,\,t$, $d_{G(s+t,0)}(x,\,u_j) > d_{G(s,t)}(x,\,u_j)$. According to the definition of π-index, we have arrived at our desired result. □

Let $T_{n,\,\triangle}$ denote the tree obtained by connecting an edge between a pendent vertex of the star $S_{\triangle+1}$ and a pendent vertex of the path $P_{n-\triangle-1}$. By repeatedly using of Lemmas 2(i) and (ii), we may arrive at the following result on trees in the end.

Theorem 6. *Among all trees of order n and maximum degree $\triangle$, the tree $T_{n,\,\triangle}$ is the unique tree having the maximum π-index.*

In particular, we have:

Corollary 4.1 ([11]). *Among all trees of order $n \geq 2$, the path P_n is the unique tree having the maximum π-index.*

Corollary 4.2 ([11]). *Among all connected graphs of order $n \geq 2$, the path P_n is the unique graph having the maximum π-index.*

Proof. Let G be a connected graph of order n with the maximum π-index. If G is a tree, then $G \cong P_n$ by Corollary 4.1. If G is a connected graph not isomorphic to a tree, then G has a spanning tree, say $T(G)$. By Proposition 1(i), we have $\pi(G) < \pi(T(G))$, a contradiction. This completes the proof. □

For $n \geq 4$, let T_n^1 be the tree obtained from the path $P_{n-1} = v_0 v_1 \dots v_{n-2}$ by attaching to v_1 a pendent edge $v_1 v_n$. By repeatedly using of Lemmas 2(i) and (ii), we can deduce the following consequence.

Theorem 7. *Among all trees of order $n \geq 4$, the tree T_n^1 is the unique tree having the second-maximum π-index.*

Recall that the factorial $n!$ is defined recursively as

$$1! = 1 \qquad 2! = 2 \qquad n! = n(n-1)!$$

for $n \geq 3$.

Gutman et al. [11] put forward the "double factorial" $n!!$ as

$$1!! = 1 \qquad 2!! = 2 \qquad n!! = n!(n-1)!!$$

for $n \geq 3$.

Here, we should note that this definition is quite different from the traditional definition for "double factorial" $n!!$.

By means of this definition for "double factorial" $n!!$, they obtained that [11]:

$$\pi(P_n) = (n-1)!!. \tag{3}$$

For $n \geq 4$, let P_n^3 be the unicyclic graph obtained from T_n^1 by connecting an edge between v_0 and v_n.

Theorem 8. *Among all unicyclic graphs of order $n \geq 5$, the graph P_n^3 is the unique unicyclic graph having the maximum π-index.*

Proof. Suppose that G is a unicyclic graph having the maximum π-index, but not isomorphic to C_n and P_n^3. Then there exists an edge e in the unique cycle of G such that $G - e$ is a tree, but $G - e \ncong P_n, T_n^1$. By Proposition 1(i) and Theorem 7, we have

$$\pi(G) \leq \frac{1}{2}\pi(G-e) < \frac{1}{2}\pi(T_n^1).$$

It can be seen that $\pi(T_n^1) = 2\pi(P_n^3)$. So, $\pi(G) < \pi(P_n^3)$, a contradiction to our choice of G. Hence, if $G \ncong C_n$, then $G \cong P_n^3$.

Now, we prove that $\pi(C_n) < \pi(P_n^3)$. Let $e = xy$ be an edge in the cycle C_n. The removal of the edge xy from C_n results in P_n. Note that $d_{C_n}(x, y) = 1$ and $d_{P_n}(x, y) = n - 1$. Similar to the proof of (i) in Proposition 1, we can verify that $\pi(C_n) < \frac{1}{n-1}\pi(P_n)$, as $n \geq 5$. Combining this and Eq. (3), $\pi(C_n) < \frac{1}{n-1}\pi(P_n) = (n-2)!(n-2)!!$. Note that $\pi(T_n^1) = 2(n-2)!\pi(P_{n-1}) = 2(n-2)!(n-2)!!$. Thus, $\pi(C_n) < \pi(P_n^3)$. This completes the proof. □

Similar to the proof of Corollary 4.2, we can prove the following result by means of Theorem 8.

Corollary 4.3. *Among all connected graphs, not isomorphic to a tree, of order $n \geq 5$, the graph P_n^3 is the unique graph having the maximum π-index.*

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