MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **85** (2021) 131-146

ISSN 0340 - 6253

On the Merrifield–Simmons Index and some Wiener–Type Indices

Hongbo Hua*, **Maolin Wang**

Faculty of Mathematics and Physics, Huaiyin Institute of Technology, 223003 Huai'an City, PR China.

(Received March 30, 2020)

Abstract

The Merrifield–Simmons index of a graph is defined to be the number of independent sets in this graph. The Wiener index of a connected graph is the total distance of this graph. These two indices are well-studied in chemical graph theory. The peripheral Wiener index and Steiner k-Wiener index are two variants of the Wiener index. In this paper, we consider the relationships between the Merrifield–Simmons index and the above-mentioned Wiener-type indices. First, we prove that the Merrifield–Simmons index is greater than peripheral Wiener index for each tree. Second, we give several sufficient conditions such that the Merrifield–Simmons index is greater than peripheral Wiener index for general connected graphs. Third, we determine sharp upper bound on the difference between the Merrifield–Simmons index and peripheral Wiener index among all trees. Finally, we establish an inequality involving the Merrifield–Simmons index, k-Steiner Wiener index and Wiener index for general connected graphs under given constraints.

1 Introduction

Throughout this paper we consider only simple connected graphs. For a graph $G = (V, E)$ with vertex set $V = V(G)$ and edge set $E = E(G)$, the *degree* of a vertex v in G, denoted by $d_G(v)$, is the number of edges incident with v. Denote by $d_G(u, v)$ the distance between vertices u and v in G. The *eccentricity* of a vertex v in a graph G is defined to be $\varepsilon_G(v) = \max\{d_G(u, v)|u \in V(G)\}$. The *diameter* of a connected graph G, denoted by $d(G)$, is equal to $\max\{\varepsilon_G(v)|v \in V(G)\}$. Let v be a vertex in G, if $\varepsilon_G(v) = d$, then v is said to be a *peripheral vertex* of G. The *periphery* of G, denoted by $\mathcal{P}(G)$, is the set of all peripheral vertices in G. Let P_n, $K_{1,n-1}$ and K_n be the path, star and complete graph of order n, respectively. The *double-star*, denoted by $S_{a,b}$ $(1 \le a, b \le n-3, a+b = n-2)$,

*Correspondence should be addressed to: hongbo_hua@163.com, hbhua@hyit.edu.cn (H. Hua).

is obtained by connecting an edge between centers of two stars S_a and S_b. For other notation and terminology not defined here, the readers are referred to [3].

Let G be a graph. A subset S of $V(G)$ is called an *independent set* of G if the subgraph induced by S contains no edges. The well-studied *Merrifield–Simmons index* (MSI) of G is defined as

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

where $i(G;k)$ denotes the number of k-membered independent sets of G for $k \geq 1$ and $i(G;0) = 1$. For results on the Merrifield–Simmons index, see e.g., [14, 15, 24–26, 29] and the references cited therein.

One of the oldest and well-studied distance-based graph invariants associated with a connected graph G is the *Wiener index*, denoted by $W(G)$, which is defined [32] as the sum of distances over all unordered vertex pairs in G, namely,

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

For results on the Wiener index, see e.g., [9, 22, 23, 30], and so on.

As a variant of Wiener index, the *peripheral Wiener index* (PWI) was introduced in [31], and is defined for a connected graph G as

$$PW(G) = \sum_{\{u,v\}\subseteq \mathcal{P}(G)} d_G(u, v).$$

For further results on the peripheral Wiener index, see [5, 20].

The *Steiner distance* $d(S)$ of a vertex subset S, which can be seen as a natural generalization of the distance between two vertices, is defined to be the minimum size of a connected subgraph whose vertex set contains S. The sum of the Steiner distances (or equivalently, the average Steiner distance) was studied earlier in [6], and was recently proposed independently as the generalization of the Wiener index [27]. For $2 \leq k \leq n$, the *Steiner k-Wiener index* $SW_k(G)$ of G is defined as

$$SW_k(G) = \sum_{S\subseteq V(G),\,|S|=k} d_G(S),$$

where $d_G(S)$ is defined as above. For recent results on the Steiner k-Wiener index, see [28, 33].

Comparing various graph invariants have gained much popularity over the past few decades, see e.g., [7, 16, 18, 19, 21–23]. Some of these researches were motivated by Grafitti conjectures [4, 8, 10] or AutoGraphiX conjectures [1, 2, 17, 18]. As a solution to a Grafitti conjecture, Chung [4] proved that the independence number is greater than or equal to average distance. Motivated by Chung's result, we naturally ask the problem: how about the relationship between the total number of independent subsets (MSI) and the total sum of peripheral distances (PWI)? Also, we consider another problem: how about the relationship between the Merrifield–Simmons index and Wiener index and Steiner Wiener index?

In this paper, our motivation is to investigate the above problems, that is, we investigate the relationships between the Merrifield–Simmons index and the above-mentioned Wiener-type indices. First, we prove that the Merrifield–Simmons index is greater than peripheral Wiener index for each tree. Second, we give several sufficient conditions such that the Merrifield–Simmons index is greater than peripheral Wiener index for general connected graphs. Third, we determine sharp upper bound on the difference between the Merrifield–Simmons index and peripheral Wiener index for each tree. Finally, we establish an inequality involving the Merrifield–Simmons index, k-Steiner Wiener index and Wiener index.

2 Main results

In this section, we investigate the relationship between the Merrifield–Simmons index and peripheral Wiener index for trees and special connected graphs. Also, we establish an inequality relating the Merrifield–Simmons index, k-Steiner Wiener index and Wiener index for general connected graphs under given constraints.

First, we find the relationship between the Merrifield–Simmons index and peripheral Wiener index. Before proceeding, we consider the following two examples.

Example 2.1. *For the complete graph K_n, we have $PW(K_n) = \frac{n(n-1)}{2} > n + 1 = i(K_n)$ for $n \geq 4$.*

Example 2.2. *For the path P_n, we have $PW(P_n) = n - 1 < n + 1 \leq i(P_n)$ for $n \geq 1$.*

Let P_5^3 be the unicyclic graph obtained by adding an edge between one vertex of C_3 and one end-vertex of P_2.

Example 2.3. *(Unicyclic graphs) For the unicyclic graph P_5^3, we have $PW(P_5^3) = 7 < 11 = i(P_5^3)$; For the cycle C_5, we have $PW(C_5) = 15 > 12 = i(C_5)$.*

Example 2.4. *(Graphs of diameter two) For* $G_1 = K_1 \oplus P_5$*, we have* $PW(G_1) = 16 > 14 = i(G_1)$*; For star* $K_{1,5}$*, we have* $PW(K_{1,5}) = 20 < 33 = i(K_{1,5})$*.*

It can be seen from the Examples 2.1-2.4 that the Merrifield–Simmons index and peripheral Wiener index are incomparable in the case of general connected graphs, even for unicyclic graphs and graphs of diameter two. So, it is natural for us to seek an explicit relationship between the the Merrifield–Simmons index and peripheral Wiener index for special connected graphs. More specially, we restrict our attention to trees and special connected graphs with given constraints.

Our first result deals with trees.

Theorem 2.1. *Let* T *be a tree. Then*

$$i(T) > PW(T).$$

Apart from trees, we also consider several special connected graph families introduced as below.

Theorem 2.2. *Let* G *be a graph with* p *peripheral vertices, diameter* d *and independence number* α*. If* $\alpha \geq \frac{\sqrt{2}}{2}pd$*, then*

$$i(G) > PW(G).$$

Theorem 2.3. *Let* G *be a graph of diameter* d *and* p *peripheral vertices. If* $p \leq \frac{\sqrt{2(d+1)}}{2}$*, then*

$$i(G) > PW(G).$$

Theorem 2.4. *Let* G *be a graph of diameter two with independence number* α *and* p *peripheral vertices. If* $\alpha \geq p$*, then*

$$i(G) > PW(G).$$

From Theorem 2.1 it follows that $i(T) - PW(T) > 0$ for any tree T. A natural problem arising at this moment is: How large is the gap between $i(G)$ and $PW(G)$ for a connected graph G?

In the following, we give a partial answer to this problem by establishing sharp upper bound on $i(T) - PW(T)$ for all trees T.

Suppose that T is a tree of order n. If $n = 2$, then $T \cong P_2$. If $n = 3$, then $T \cong P_3$. So, we assume that $n \geq 4$. Our result reads as follows.

Theorem 2.5. *Let T be a tree of order $n \geq 4$.*

(1) *If $n = 4$, then*

$$i(T) - PW(T) \leq 5$$

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

(2) *If $5 \leq n \leq 7$, then*

$$i(T) - PW(T) \leq 9 \cdot 2^{n-5}$$

with equality if and only if $T \cong T^*$, where T^* is the tree obtained by attaching $n-5$ pendent edges to the middle-point of the path P_5;

(3) *If $n \geq 8$, then*

$$i(T) - PW(T) \leq 2^{n-1} - n^2 + 3n - 1$$

with equality if and only if $T \cong K_{1,n-1}$.

Besides Theorems 2.1-2.5, we also establish an inequality involving the Merrifield–Simmons index, k-Steiner Wiener index and Wiener index. This result is stated as follows.

Theorem 2.6. *Let G be a connected graph of order n and size m. For each positive integer $3 \leq k \leq n-1$, if $m \leq \frac{n^2+n+2}{2} - \frac{2(n-1)(n-2)\cdots(n-k+1)}{k!}$, then*

$$i(G) > \frac{SW_k(G)}{W(G)} .$$

In particular, when $k = 3$, by Theorem 2.6, we obtain the following result.

Corollary 2.7. *Let G be a connected graph of order $n \geq 4$ and size m. If $m \leq \frac{n^2+9n+2}{6}$, then*

$$i(G) > \frac{SW_3(G)}{W(G)} .$$

Let G be a connected graph of order n and size m. If G is a tree, then $m = n-1$; if G is a unicyclic graph, then $m = n$; and if G is a bicyclic graph, then $m = n+1$. So, by Corollary 2.7, we have the following results.

Corollary 2.8. *Let T be a tree of order $n \geq 4$. Then*

$$i(T) > \frac{SW_3(T)}{W(T)} .$$

Corollary 2.9. *Let G be a unicyclic graph of order $n \geq 4$. Then*

$$i(G) > \frac{SW_3(G)}{W(G)} .$$

Corollary 2.10. *Let G be a bicyclic graph of order $n \geq 4$. Then*

$$i(G) > \frac{SW_3(G)}{W(G)} .$$

3 Proofs of Theorems 2.1–2.6

In this section, we give the proofs of Theorems 2.1–2.6.

First, we prove Theorem 2.1. Before proceeding, we introduce some preliminary results.

Lemma 3.1. *Suppose that T is a tree of diameter d and p peripheral vertices with independence number α. Then*

$$\alpha \;\geq\; \left\lceil \frac{d+1}{2} \right\rceil + (p-2). \tag{1}$$

Moreover, the lower bound is sharp as shown by the star, double-star, and the path.

Proof. If $d = 2$, then $p = n-1$, $\alpha = n-1 = \lceil \frac{d+1}{2} \rceil + (p-2)$. If $d = 3$, then T is a double-star, and $p = n-2$, $\alpha = n-2 = \lceil \frac{d+1}{2} \rceil + (p-2)$. If $d = n-1$, then $p = 2$, $\alpha = \lceil \frac{n}{2} \rceil = \lceil \frac{d+1}{2} \rceil + (p-2)$. So, we assume that $4 \leq d \leq n-2$.

Let $P_{d+1} = v_1 v_2 \ldots v_d v_{d+1}$ be a diametrical path in T. First, we take a maximum independent set S of P_{d+1} as follows:

- If d is odd, then we let $S = \{v_1, v_3, v_5, \ldots, v_{d-2}, v_{d+1}\}$;
- If d is even, then we let $S = \{v_1, v_3, v_5, \ldots, v_{d-1}, v_{d+1}\}$.

If $p = 2$, then $\alpha = \alpha(G) \geq \alpha(P_{d+1}) = \lceil \frac{d+1}{2} \rceil = \lceil \frac{d+1}{2} \rceil + (p-2)$, as desired. So, we suppose that $p \geq 3$. Let $\mathcal{P}(T) = \{v_1, v_{d+1}, u_1, \ldots, u_{p-2}\}$. Clearly, $u_s \in V(T) \setminus V(P_{d+1})$ and $d_T(u_s) = 1$ for each $s = 1, \ldots, p-2$. According to the definition of peripheral vertex, we have: if d is odd, then $u_s v_t \notin E(T)$ for each $s = 1, \ldots, p-2$ and $t = 1, 3, 5, \ldots, d-2, d+1$; if d is even, then $u_s v_t \notin E(T)$ for each $s = 1, \ldots, p-2$ and $t = 1, 3, 5, \ldots, d-1, d+1$. Thus, by the above chosen S, we construct an independent set S' of T as follows:

- If d is odd, then we let $S' = \{v_1, v_3, \ldots, v_{d-2}, v_{d+1}, u_1, \ldots, u_{p-2}\}$;
- If d is even, then we let $S' = \{v_1, v_3, \ldots, v_{d-1}, v_{d+1}, u_1, \ldots, u_{p-2}\}$.

So, according to the definition of independence number, when d is odd, we have

$$\alpha \geq |S'| = \frac{d+1}{2} + (p-2) = \left\lceil \frac{d+1}{2} \right\rceil + (p-2),$$

when d is even, we have

$$\alpha \geq |S'| = \frac{d}{2} + 1 + (p-2) = \left\lceil \frac{d+1}{2} \right\rceil + (p-2).$$

It is easy to check that the star, double-star, and the path attain the lower bound in (1). This completes the proof. ■

Lemma 3.2. *Suppose that G is a connected graph of order n with independence number α. Then*

$$i(G) > 2^{\alpha} .$$

Proof. Let S be an independent set of G with $|S| = \alpha$. Clearly $\alpha \geq 1$. If $G - S = K_1$, then $G \cong K_{1,n-1}$, as G is connected. It is easy to check that $i(G) = 2^{n-1} + 1 > 2^{n-1} = 2^{\alpha}$. So, we assume that $|G - S| \geq 2$. Note that adding edges into $G - S$ will strictly decrease the Merrifield–Simmons index of G. Then $i(G) \geq i(\alpha K_1 \oplus K_{n-\alpha}) = 2^{\alpha} + n - \alpha > 2^{\alpha}$. ■

By means of Lemmas 3.1 and 3.2, we obtain a lower bound on the Merrifield–Simmons index of trees.

Proposition 3.3. *Suppose that T is a tree of diameter d and p peripheral vertices. Then*

$$i(T) > 2^{\lceil \frac{d+1}{2} \rceil + (p-2)} . \tag{2}$$

Next, we give an upper bound for peripheral Wiener index of general connected graphs.

Lemma 3.4. *Suppose that G is a connected graph of diameter d and p peripheral vertices. Then*

$$PW(G) \leq \binom{p}{2} d . \tag{3}$$

Moreover, the upper bound is sharp as shown by the star and the path.

Proof. Since $d_G(x, y) \leq d$ holds for any one pair of peripheral vertices x and y in G, we have

$$PW(G) \leq \binom{p}{2} d .$$

It is easy to check that the star and the path attain the upper bound in (3). ■

The following result is easy to obtain, and its proof is omitted here.

Lemma 3.5. *For any positive real number $x > 4$, it holds that*

$$2^x > x^2 \ .$$

Now, we are in a position to prove Theorem 2.1.

The proof of Theorem 2.1

Proof. Let n and d be the order and diameter of T, respectively. Denote by $\mathcal{P}(T)$ the set of peripheral vertices in T and let $|\mathcal{P}(T)| = p$. Obviously $p \geq 2$. If $n = 2$, then $T \cong P_2$, and $i(P_2) = 3 > 1 = PW(P_2)$. So, we assume that $n \geq 3$.

When $d = 2$, we have $T \cong K_{1,\,n-1}$. When $d = 3$, we have $T \cong S_{a,\,b}$ $(1 \leq a,\, b \leq n-3,$ $a + b = n - 2)$. An elementary calculation gives $i(K_{1,\,n-1}) = 2^{n-1} + 1 > (n-1)(n-2) = PW(K_{1,\,n-1})$, $i(S_{a,\,b}) = 2^{a+b} + 2^a + 2^b > (a+b)^2 + (a-1)(b-1) - 1 = PW(S_{a,\,b})$ for each $1 \leq a,\, b \leq n-3$ and $a + b = n - 2$.

Because for any connected graph G, we have $i(G) \geq n + 1 = i(K_n)$ with equality if and only if $G \cong K_n$. So, for a tree T, $i(T) > n + 1$. If $p = 2$, then $PW(T) = d \leq n - 1$. So, $i(T) > PW(T)$.

Now, we assume that $d \geq 4$ and $p \geq 3$. By (2) and (3), we have

$$i(T) - PW(T) > 2^{\lceil \frac{d+1}{2} \rceil + (p-2)} - \binom{p}{2} d \ . \tag{4}$$

Note that $2^{\lceil \frac{d+1}{2} \rceil} \geq d$ for any positive integer d. Moreover, when $p \geq 6$, by Lemma 3.5, we have $2^{(p-2)} - \binom{p}{2} \geq (p-2)^2 - \frac{p(p-1)}{2} = \frac{1}{2}(p^2 - 7p + 8) > 0$. So, by (4), $i(T) > PW(T)$ holds for $p \geq 6$.

In the following, we consider the remaining case of $3 \leq p \leq 5$. Let $f(d,\, p) = 2^{\lceil \frac{d+1}{2} \rceil + (p-2)} - \binom{p}{2} d$.

When $p = 3$, we have $f(d,\, 3) = 2^{\lceil \frac{d+1}{2} \rceil + 1} - 3d$. By our assumption that $d \geq 4$, we have $\lceil \frac{d+1}{2} \rceil \geq 3$, and thus, $\lceil \frac{d+1}{2} \rceil + 1 \geq 4$. According to Lemma 3.5, we have $f(d,\, 3) = 2^{\lceil \frac{d+1}{2} \rceil + 1} - 3d \geq \left(\lceil \frac{d+1}{2} \rceil + 1 \right)^2 - 3d \geq \left(\frac{d+1}{2} + 1 \right)^2 - 3d = \frac{1}{4}(d^2 - 6d + 9) > 0$.

When $p = 4$, we have $f(d,\, 4) = 2^{\lceil \frac{d+1}{2} \rceil + 2} - 6d = 2f(d,\, 3) > 0$.

When $p = 5$, we have $f(d,\, 5) = 2^{\lceil \frac{d+1}{2} \rceil + 3} - 10d = 4\left(2^{\lceil \frac{d+1}{2} \rceil + 1} - 3d\right) + 2d = 4f(d,\, 3) + 2d > 0$.

So, by (4), $i(T) > PW(T)$ holds for $3 \leq p \leq 5$. Summarizing above, we have completed the proof. ■

The proof of Theorem 2.2

Proof. Let n be the order of G. Then $n \geq p \geq 2$. If $\alpha = 1$, then $G \cong K_n$ and $\frac{\sqrt{2}}{2}pd = \frac{\sqrt{2}}{2}n > 1 = \alpha$, a contradiction to our assumption. If $\alpha = 2$, noting that $p \geq 2$ and $\alpha \geq \frac{\sqrt{2}}{2}pd$, we have $d = 1$, thus $G \cong K_n$, a contradiction. If $\alpha = 3$, noting that $p \geq 2$ and $\alpha \geq \frac{\sqrt{2}}{2}pd$, we have $d \leq 2$. Since $\alpha = 3$, we also have $d \geq 2$. So, $d = 2$. Also, we have $p = 2$, for otherwise, $\frac{\sqrt{2}}{2}pd > \alpha$, a contradiction. Let x be a vertex in G such that $\varepsilon_G(x) = 2$, and y be the unique vertex in G such that $d_G(x, y) = \varepsilon_G(x)$. Set $V_x(i) = \{v \in V(G) | d_G(x, v) = i\}$, $i = 1, 2$. Then $|V_x(2)| = |\{y\}| = 1$, and $|V_x(1)| = n-2$. Since $p = 2$, we have $\varepsilon_G(v) = 1$ for each $v \in V_x(1)$. So, $d_G(v) = n-1$ for each $v \in V_x(1)$. Thus, $\alpha = 2$, a contradiction. Now, we assume that $\alpha \geq 4$. By Lemmas 3.2, 3.4, 3.5 and our assumption that $\alpha \geq \frac{\sqrt{2}}{2}pd$, we have

$$i(G) - PW(G) \;>\; 2^\alpha - \binom{p}{2}d \geq \alpha^2 - \frac{p(p-1)}{2}d \geq \frac{p^2d^2}{2} - \frac{p(p-1)}{2}d > 0\ .$$

This completes the proof. ■

The proof of Theorem 2.3

Proof. Let P_{d+1} be a diametrical path in G. Clearly, we have $\alpha = \alpha(G) \geq \alpha(P_{d+1}) \geq \lceil \frac{d+1}{2} \rceil$.

Since $2 \leq p \leq \frac{\sqrt{2(d+1)}}{2}$, we have $d+1 \geq 8$, that is, $\frac{d+1}{2} \geq 4$. So, by Lemmas 3.2, 3.4, 3.5 and our assumption that $p \leq \frac{\sqrt{2(d+1)}}{2}$, we have

$$\begin{aligned} i(G) - PW(G) \;&>\; 2^\alpha - \binom{p}{2}d \geq 2^{\lceil \frac{d+1}{2} \rceil} - \frac{p(p-1)}{2}d \geq 2^{\frac{d+1}{2}} - \frac{p(p-1)}{2}d \\ &>\; 2^{\frac{d+1}{2}} - \frac{p^2}{2}d \geq \left(\frac{d+1}{2}\right)^2 - \frac{\left(\frac{\sqrt{2(d+1)}}{2}\right)^2}{2}d > 0\ . \end{aligned}$$

This completes the proof. ■

The proof of Theorem 2.4

Proof. Let n and d be the order and diameter of G, respectively. Obviously $p \geq 2$. If $n = 2$, then by Lemmas 3.2 and 3.4 and our assumption that $\alpha(G) \geq p$ and $d = 2$, we have

$$i(G) - PW(G) > 2^\alpha - \binom{p}{2}d \geq 2^p - p^2 + p. \tag{5}$$

Let $f(p) = 2^p - p^2 + p$. If $p = 2$ or $p = 3$, by (5), we have $i(G) - PW(G) > f(p) > 0$. Now, we assume that $p \geq 4$. It is easy to obtain that $\frac{df(p)}{dp} = 2^p \ln 2 - 2p + 1 > 2^{p-1} - 2p + 1$ and that $\frac{d^2 f(p)}{dp^2} = 2^p (\ln 2)^2 - 2 = 2^{p-2}(2\ln 2)^2 - 2 > 2^{p-2} - 2$. When $p \geq 3$, we have $\frac{d^2 f(p)}{dp^2} > 0$. So, $\frac{df(p)}{dp}$ is a strictly increasing function on the interval $[3, +\infty]$. Note that $\frac{df(p)}{dp}|_{p=4} = 1 > 0$. So, $f(p)$ is a strictly increasing function on the interval $[4, +\infty]$. Thus, by (5), we have $i(G) - PW(G) > f(p) > f(4) = 4 > 0$. This completes the proof. ∎

The proof of Theorem 2.5

We first give some preliminary results.

Lemma 3.6 ([13]). *Let G be a graph. If x is a vertex in G, then $i(G) = i(G-x) + i(G - N_G[x])$.*

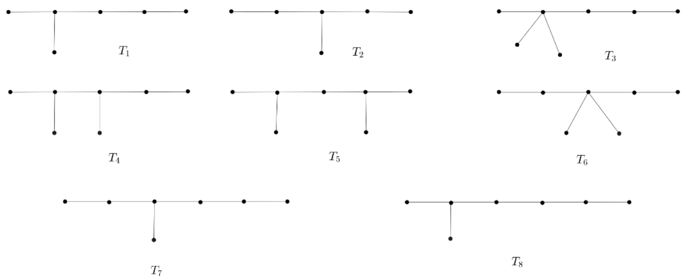

Figure 1: Trees T_i $(1 \leq i \leq 8)$ occurred in the proof of Theorem 2.5.

Table 1

T	$i(T) - PW(T)$
P_5	11
P_6	19
P_7	32
T_1	13
T_2	18
T_3	25
T_4	28
T_5	21
T_6	36
T_7	31
T_8	25

The values of $i(T) - PW(T)$ for trees of small order n $(5 \leq n \leq 7)$.

Let F_n be the nth Fibonacci number, i.e., $F_0 = F_1 = 1$, $F_n = F_{n-1} + F_{n-2}$, $n \geq 2$. In 2007, Liu et al. obtained a result on the Merrifield–Simmons index for trees with given diameter.

Theorem 3.7 ([29]). *Let T be a tree on n vertices with diameter d. Then*

$$i(T) \leq F_{d+2} + (2^{n-d-1} - 1)F_2F_d$$

with equality if and only if $G \cong W_{n,\,d,\,1}$, where $W_{n,\,d,\,1}$ is the tree of diameter d obtained by attaching $n-d-1$ pendent vertices to v_1 (or v_{d-1}) of the path $P_{d+1} = v_0v_1 \cdots v_{d-1}v_d$.

By the definition of $W_{n,\,d,\,1}$ and properties of Fibonacci number, we obtain the following result.

Lemma 3.8. *For $d \geq 4$, we have $i(W_{n,\,d,\,1}) \leq i(W_{n,\,4,\,1})$ with equality if and only if $d = 4$.*

By Theorem 3.7 and Lemma 3.8, we get sharp upper bound on the Merrifield–Simmons index for trees of diameter no less than four.

Theorem 3.9. *Let T be a tree of order n with diameter $d \geq 4$. Then*

$$i(T) \leq 5 \cdot 2^{n-4} + 3$$

with equality if and only if $T \cong W_{n,\,4,\,1}$.

Now, we give the proof of Theorem 2.5.

Proof. When $n = 4$, we have $T \cong P_4$ or $K_{1,3}$. It is easy to obtain that $i(P_4) - PW(P_4) = 5 > 3 = i(K_{1,3}) - PW(K_{1,3})$. Therefore, (1) holds. So, we assume that $n \geq 5$.

Let d be the diameter of T. If $d = 2$, then $T \cong K_{1,\,n-1}$. Clearly, $i(K_{1,\,4}) - PW(K_{1,\,4}) = 5$, $i(K_{1,\,5}) - PW(K_{1,\,5}) = 13$, $i(K_{1,\,6}) - PW(K_{1,\,6}) = 35$. From Table 1, we conclude that for $5 \leq n \leq 7$, we have $i(K_{1,\,n-1}) - PW(K_{1,\,n-1}) < i(T^*) - PW(T^*)$. So, we assume that $n \geq 8$.

Since $i(K_{1,\,n-1}) - PW(K_{1,\,n-1}) = 2^{n-1} - n^2 + 3n - 1$ and $i(T^*) - PW(T^*) = 9 \cdot 2^{n-5}$, we have $(i(K_{1,\,n-1}) - PW(K_{1,\,n-1})) - (i(T^*) - PW(T^*)) = 7 \cdot 2^{n-5} - n^2 + 3n - 1$. Let $f(x) = 7 \cdot 2^{x-5} - x^2 + 3x - 1$. Then $\frac{df(x)}{dx} = 7 \ln 2 \cdot 2^{x-5} - 2x + 3 > 2 \cdot 2^{x-5} - 2x + 3 = 2^{x-4} - 2x + 3$. Let $g(x) = 2^{x-4} - 2x + 3$. Then $\frac{dg(x)}{dx} = 2 \ln 2 \cdot 2^{x-5} - 2 > 2^{x-5} - 2$. For $x \geq 6$, we have $\frac{dg(x)}{dx} > 0$. So, $g(x)$ is a strictly increasing function on the interval $[6, +\infty)$. Then $g(x) \geq g(8) = 3 > 0$. Therefore, when $x \geq 8$, we have $\frac{df(x)}{dx} > g(x) > 0$, that is, $f(x)$ is a strictly increasing function on the interval $[8, +\infty)$. Then $f(x) > f(8) = 15 > 0$. Now, for $n \geq 8$, we have $(i(K_{1,n-1}) - PW(K_{1,n-1})) - (i(T^*) - PW(T^*)) \geq f(n) > 0$. That is, $i(K_{1,n-1}) - PW(K_{1,n-1}) > i(T^*) - PW(T^*)$ for $n \geq 8$.

Next, we assume that $d \geq 3$. We consider the following two cases.

Case 1. $d = 3$.

In this case, T is a double-star, that is, $T \cong S_{a,b}$ ($1 \leq a, b \leq n-3$ and $a+b = n-2$). By Lemma 3.6, we have $i(T) = 2^{a+b} + 2^a + 2^b = 2^{n-2} + 2^a + 2^b$ and $PW(T) = a^2 + b^2 + 3ab - a - b = (a+b)^2 + (a-1)(b-1) - 1 = (n-2)^2 + (a-1)(b-1) - 1$. When $n = 5$, we have $(i(S_{1,2}) - PW(S_{1,2})) - (i(T^*) - PW(T^*)) = (i(S_{1,2}) - PW(S_{1,2})) - (i(P_5) - PW(P_5)) = 8 - 11 < 0$, that is, $i(S_{1,2}) - PW(S_{1,2}) < i(T^*) - PW(T^*)$.

Now, we assume that $n \geq 6$. If $\min\{a, b\} = 1$, then $i(T) - PW(T) = (2^{n-2} + 2^{n-3} + 2) - [(n-2)^2 - 1] = 3 \cdot 2^{n-3} - n^2 + 4n - 1$. So, $(i(K_{1,n-1}) - PW(K_{1,n-1})) - (i(T) - PW(T)) = 2^{n-3} - n > 0$ as $n \geq 6$. Thus, we may assume that $\min\{a, b\} \geq 2$. Then $2 \leq a, b \leq n-4$. Therefore,

$$\begin{aligned} i(T) - PW(T) &= (2^{n-2} + 2^a + 2^b) - [(n-2)^2 + (a-1)(b-1) - 1] \\ &< (2^{n-2} + 2^a + 2^b) - (n-2)^2 + 1 \leq 2^{n-2} + 2 \cdot 2^{n-4} - (n-2)^2 + 1 \\ &\leq 3 \cdot 2^{n-3} - (n-2)^2 + 1 < 2^{n-1} - n^2 + 3n - 1 \\ &= i(K_{1,n-1}) - PW(K_{1,n-1}). \end{aligned}$$

So, for $n \geq 6$, we have $i(K_{1,n-1}) - PW(K_{1,n-1}) > i(T) - PW(T)$. In particular, by our previous proof, for $5 \leq n \leq 7$, we have $i(T^*) - PW(T^*) > i(K_{1,n-1}) - PW(K_{1,n-1}) > i(T) - PW(T)$.

Case 2. $d \geq 4$.

If $5 \leq n \leq 7$, then T must be isomorphic to P_5, or P_6, or P_7, or T_i ($1 \leq i \leq 8$), see Fig. 1. It is easy to check from Table 1 that $i(T) - PW(T) < i(T^*) - PW(T^*)$ holds. Now, we assume that $n \geq 8$. By Theorem 3.9, we have $i(T) \leq 5 \cdot 2^{n-4} + 3$. Also, $PW(T) \geq 4$. So, $i(T) - PW(T) \leq 5 \cdot 2^{n-4} - 1$. Let $f(x) = 2^{x-1} - x^2 + 3x - 1 - 5 \cdot 2^{x-4} + 1 = 3 \cdot 2^{x-4} - x^2 + 3x$. Then $\frac{df(x)}{dx} = 3 \ln 2 \cdot 2^{x-4} - 2x + 3 > 2^{x-4} - 2x + 3$. Let $g(x) = 2^{x-4} - 2x + 3$. Similar to the case of $d = 2$, we can prove that $(i(K_{1,n-1}) - PW(K_{1,n-1})) - (i(T) - PW(T)) \geq f(n) > 0$ for $n \geq 8$, that is, $i(K_{1,n-1}) - PW(K_{1,n-1}) > i(T) - PW(T)$ for $n \geq 8$.

Summarizing above, we have completed the proof. ■

In the following, we prove Theorem 2.6. We first give a lower bound, in terms of order and size, for the Merrifield–Simmons index of general graphs.

Theorem 3.10. *Let G be a connected graph of order n and size m. Then*

$$i(G) \geq \frac{n^2+n+2}{2} - m \; . \tag{6}$$

Proof. Let $\alpha(G)$ be the independence number of G. If $G \cong K_n$, then $m = \frac{n(n-1)}{2}$ and $i(K_n) = n+1$, the equality (6) holds. Now, we assume that $G \ncong K_n$.

Since $G \ncong K_n$, we have $\alpha(G) \geq 2$. Let $i(G; u; 2)$ be the number of 2-independent sets containing u in G. Then $i(G; u; 2) = n - d_G(u) - 1$. So,

$$\begin{aligned} i(G) &\geq 1 + n + i(G; 2) = 1 + n + \frac{1}{2} \sum_{u \in V(G)} i(G; u; 2) \\ &= 1 + n + \frac{1}{2} \sum_{u \in V(G)} (n - d_G(u) - 1) = \frac{n^2+n+2}{2} - m \, , \end{aligned}$$

as expected. ■

The proof of Theorem 2.6.

Proof. By the definition of k-Steiner Wiener index, we have

$$\begin{aligned} SW_k(G) &= \sum_{S \subseteq V(G),\, |S|=k} d_G(S) \leq (n-1)\binom{n}{k} = \frac{(n-1)n(n-1)\cdots(n-k+1)}{k!} \\ &= \frac{n(n-1)}{2} \cdot \frac{2(n-1)\cdots(n-k+1)}{k!} \leq W(G) \cdot \frac{2(n-1)\cdots(n-k+1)}{k!} \\ & \qquad\qquad \left(\text{as } W(G) \geq W(K_n) = \tfrac{n(n-1)}{2}\right) \end{aligned} \tag{7}$$

By Theorem 3.10, (7) and our assumption that $m \leq \frac{n^2+n+2}{2} - \frac{2(n-1)(n-2)\cdots(n-k+1)}{k!}$, we have

$$\begin{aligned} i(G) \cdot W(G) &\geq \left[\frac{n^2+n+2}{2} - \frac{n^2+n+2}{2} + \frac{2(n-1)(n-2)\cdots(n-k+1)}{k!}\right] \cdot \\ & \quad \frac{k!}{2(n-1)(n-2)\cdots(n-k+1)} SW_k(G) = SW_k(G), \end{aligned}$$

that is, $i(G) \geq \frac{SW_k(G)}{W(G)}$.

Note that $k \geq 3$ and $m \leq \frac{n^2+n+2}{2} - \frac{2(n-1)(n-2)\cdots(n-k+1)}{k!}$. Thus, $G \ncong K_n$. So, the equality in (7) can not be attained, and then $i(G) > \frac{SW_k(G)}{W(G)}$.

This completes the proof. ■

4 Concluding remarks

In this paper, we investigated the relationships between the Merrifield–Simmons index some Wiener-type indices. We first proved that the Merrifield–Simmons index is greater than the peripheral Wiener index for all trees. Also, we gave several sufficient conditions such that the Merrifield–Simmons index is greater than peripheral Wiener index for general connected graphs. Moreover, we determined sharp upper bound on the difference between the Merrifield–Simmons index and peripheral Wiener index for all trees. Furthermore, we established an inequality relating the Merrifield–Simmons index, k-Steiner Wiener index and Wiener index. We end the paper by proposing the following problems.

Problem 4.1. *Determine general connected graph or special connected graph G such that the inequalities*

$$i(G) > PW(G)$$

or

$$i(G) < PW(G)$$

hold.

Problem 4.2. *Determine sharp lower and upper bounds on the difference $i(G) - PW(G)$ for general connected graph G.*

Acknowledgments: This research was supported by National Natural Science Foundation of China under Grant Nos. 11971011, 11571135, and sponsored by Qing Lan Project of Jiangsu Province, P.R. China.

References

[1] M. Aouchiche , J. M. Bonnefoy , A. Fidahoussen, G. Caporossi, P. Hansen, L. Hiesse, J. Lachere, A. Monhait, Variable neighborhood search for extremal graphs. 14. The autoGraphiX 2 system, in: L. Liberti, N. Maculan (Eds.), *Global Optimization: From Theory to Implementation*, Springer, New York, 2006, pp. 281–310.

[2] M. Aouchiche, P. Hansen, Proximity and remoteness in graphs: results and conjectures, *Networks* **58** (2011) 95–102.

[3] J. A. Bondy, U. S. R. Murty, *Graph Theory with Applications*, Macmillan, London, 1976.

[4] F. R. K. Chung, The average distance and the independence number, *J. Graph Theory* **12** (1988) 229–235.

[5] Y. H. Chen, H. Wang, X. D. Zhang, Peripheral Wiener index of trees and related questions, *Discr. Appl. Math.* **251** (2018) 135–145.

[6] P. Dankelmann, O. R. Oellermann, H. C. Swart, The average Steiner distance of a graph, *J. Graph Theory* **22** (1996) 15–22.

[7] K. C. Das, I. Gutman, On Wiener and multiplicative Wiener indices of graphs, *Discr. Appl. Math.* **206** (2016) 9–14.

[8] E. DeLaViña, B. Waller, Spanning trees with many leaves and average distance, *El. J. Comb.* **15** (2008) #R33.

[9] A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and applications, *Acta Appl. Math.* **66** (2001) 211–249.

[10] S. Fajtlowicz, W. A. Waller, On two conjectures of GRAFFITI II, *Congr. Num.* **60** (1987) 187–197.

[11] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.

[12] I. Gutman, W. Linert, I. Lukovits, Ž. Tomović, On the multiplicative Wiener index and its possible chemical applications, *Monatsh. Chem.* **131** (2000) 421–427.

[13] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer, Berlin, 1986.

[14] H. Hua, A sharp upper bound for the number of stable sets in graphs with given number of cut edges, *Appl. Math. Lett.* **22** (2009) 1380–1385.

[15] H. Hua, S. Zhang, Graphs with given number of cut vertices and extremal Merrifield–Simmons index, *Discr. Appl. Math.* **159** (2011) 971–980.

[16] H. Hua, K. C. Das, The relationship between the eccentric connectivity index and Zagreb indices, *Discr. Appl. Math.* **161** (2013) 2480–2491.

[17] H. Hua, K. C. Das, Proof of conjectures on remoteness and proximity in graphs, *Discr. Appl. Math.* **171** (2014) 72–80.

[18] H. Hua, Y. Chen, K. C. Das, The difference between remoteness and radius of a graph, *Discr. Appl. Math.* **187** (2015) 103–110.

[19] H. Hua, H. Wang, X. Hu, On eccentric distance sum and degree distance of graphs, *Discr. Appl. Math.* **250** (2018) 262–275.

[20] H. Hua, On the peripheral Wiener index of graphs, *Discr. Appl. Math.* **258** (2019) 135–142.

[21] H. Hua, Comparing multiplicative Wiener index with other graph invariants, *MATCH Commun. Math. Comput. Chem.* **83** (2020) 95–107.

[22] S. Klavžar, M. J. Nadjafi–Arani, Wiener index in weighted graphs via unification of Θ^*-classes, *Eur. J. Comb.* **36** (2014) 71–76.

[23] S. Klavžar, M. J. Nadjafi–Arani, Improved bounds on the difference between the Szeged index and the Wiener index of graphs, *Eur. J. Comb.* **39** (2014) 148–156.

[24] S. Li, X. Li, W. Jing, On the extremal Merrifield–Simmons index and Hosoya index of quasi–tree graphs, *Discr. Appl. Math.* **157** (2009) 2877–2885.

[25] S. Li, Z. Zhu, The number of independent sets in unicyclic graphs with a given diameter, *Discr. Appl. Math.* **157** (2009) 1387–1395.

[26] X. Li, H. Zhao, I. Gutman, On the Merrifield–Simmons index of trees, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 389–402.

[27] X. Li, Y. Mao, I. Gutman, The Steiner Wiener index of a graph, *Discuss. Math. Graph Theory* **36** (2016) 455–465.

[28] X. Li, Y. Mao, I. Gutman, Inverse problem on the Steiner Wiener index, *Discuss. Math. Graph Theory* **38** (2018) 83–95.

[29] H. Liu, X. Yan, Z. Yan, On the Merrifield–Simmons indices and Hosoya indices of trees with a prescribed diameter, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 371–384.

[30] S. Mukwembi, T. Vetrik, Wiener index of trees of given order and diameter at most 6, *Bull. Aust. Math. Soc.* **89** (2014) 379–396.

[31] K. P. Narayankar, S. B. Lokesh, Peripheral Wiener index of a graph, *Commun. Comb. Opt.* **2** (2017) 43–56.

[32] H. Wiener, Structural determination of paraffin boiling point, *J. Amer. Chem. Soc.* **69** (1947) 17–20.

[33] J. Zhang, H. Wang, X. D. Zhang, The Steiner Wiener index of trees with a given segment sequence, *Appl. Math. Comput.* **344-345** (2019) 20–29.