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Relations between Merrifield–Simmons and Wiener Indices

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Abstract

The Merrifield–Simmons index $i(G)$ of a graph G is defined as the total number of the independent vertex sets (including the empty vertex set) in G and the Wiener index $W(G)$ is the sum of the distances in all unordered pairs of vertices of G. Motivated by the recent work [H. Hua, M. Wang, On the Merrifield–Simmons index and some Wiener-type indices, *MATCH Commun. Math. Comput. Chem.* **85** (2021) in press], we characterize some relations between $i(G)$ and $W(G)$ for connected graphs. It is shown that $i(G) > W(G)$ for any graph G of order $n \geq 11$ with m edges where $n-1 \leq m \leq n+1$. Moreover, some relations between $i(G)$ and $W(G)$ are obtained for graphs with diameter 2 and Cartesian products of graphs. In particular, we prove that $i(G \,\Box\, P_2) > W(G \,\Box\, P_2)$ for any connected bipartite graph G of order at least 54 and $i(G \,\Box\, S_n) > W(G \,\Box\, S_n)$ for any connected graph G and star S_n with $n \geq 6$.

1 Introduction

All graphs considered in this paper are finite, undirected and simple. If $G = (V(G), E(G))$ is a graph, we will use $n(G) = |V(G)|$ for its order and $m(G) = |E(G)|$ for its size. The *degree* $\deg_G(v)$ of $v \in V(G)$ is the number of vertices in G adjacent to v. We denote by $N_G(v)$ the *open neighborhood* of vertex v in G. For two vertices $u, v \in V(G)$, we use $d_G(u, v)$ to denote the distance between u and v in the graph G. The *eccentricity* $\varepsilon_G(v)$ of a vertex $v \in V(G)$ is the maximum distance among all distances from the vertex v to any other vertex of G. If $\varepsilon_G(v) = k$ for any vertex $v \in V(G)$, then G is *k-self-centered.* The complement of G is denoted with $\overline{G}$. We denote by S_n, P_n and K_n the star, the path and the complete graph on n vertices, respectively, throughout this paper. Other undefined notations and terminology on the graph theory can be found in [1].

A graph invariant is a function from the set of graphs to the reals which is invariant under graph automorphisms, which is known as topological index in chemical graph theory. The Merrifield–Simmons index of a graph G, denoted by $i(G)$ and introduced in [19], is defined as the total number of independent vertex sets, including the empty vertex set of G.

$$i(G) = \sum_{i=0}^{\alpha(G)} i(G,k)$$

where $i(G,k)$ with $k \in \{0,1,2,\ldots,\alpha(G)\}$ denotes the number of k-independent sets in G and $\alpha(G)$ is the *independence number* of G.

Let F_n be the nth Fibonacci number, that is, $F_0 = 0$, $F_1 = 1$ and $F_n = F_{n-1}+F_{n-2}$ for $n \geq 2$. The Merrifield–Simmons index is also called Fibonacci number of a graph mainly for the reason that $i(P_n) = F_{n+2}$. For some more results on the Merrifield–Simmons index, see [4, 5, 28, 33] and a survey [26] with references therein.

The oldest topological index in chemical graph theory is the Wiener index [27] (with the multiplicative version of it, see [3, 13]). It is still attracting the interest of scientists, cf. [6, 16–18, 30, 32] and is defined as

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

As a variant of Wiener index, the peripheral Wiener index introduced in [20] is just $PW(G) = \sum_{\{u,v\}\subseteq \mathcal{P}(G)} d_G(u,v)$ for a connected graph G where $\mathcal{P}(G)$ denotes the *periphery*, that is, the set of vertices with maximum eccentricity, of G.

Throughout this paper we use the notation $[k] = \{1,2,\ldots,k\}$ for any positive integer k. The *join* of two vertex–disjoint graphs G and H, denoted by $G \oplus H$, is a graph with vertex set $V(G)\bigcup V(H)$ and edge set $\{uv | u \in V(G), v \in V(H)\}\bigcup E(G)\bigcup E(H)$. The *Cartesian product* $G\Box H$ of vertex–disjoint graphs G and H is the graph with $V(G\Box H) = V(G) \times V(H)$ and (g,h) is adjacent to (g',h') if either $gg' \in E(G)$ and $h = h'$, or $g = g'$ and $hh' \in E(H)$. Some mathematical properties of the Cartesian products of two graphs can be found in [22].

Recently the comparative study between two invariants of graphs has attracted the attention of some chemical and mathematical researchers. Furtula, et al. [9] reported some comparison results between vertex–degree–based invariants of (molecular) graphs. Hua, et al. [14, 15] compared the Merrifield–Simmons index with some distance–based invariants of graphs. Some other results of this type can be seen in [29–31].

In this paper we continue the research in this direction by comparing the Merrifield–Simmons index with the Wiener index of connected graphs. In the next section we list or prove some preliminary results for the use in subsequent proofs. Results on the comparison of the Merrifield–Simmons and Wiener indices for the sparse graphs and graphs with diameter 2 are given in in Section 3. In Section 4 we construct some more graphs with property $i(G) > W(G)$, by using the tool of Cartesian products of graphs. Moreover, several related open problems are proposed in Section 5 to the comparison between i and W.

2 Preliminaries

To obtain our main results, we first give some lemmas as necessary preliminaries.

Lemma 2.1. ([26]) *Let G be a graph. Then*

(i) $i(G) = i(G - v) + i(G - N_G[v])$ *for* $v \in V(G)$*;*

(ii) $i(G) = \prod_{k=1}^{t} i(G_k)$ *if* G_1, $G_2, \cdots$, G_t *are the components of graph* G*.*

Denote by $C_k(n_1^{l_1}, n_2^{l_2}, ..., n_m^{l_m})$ the unicyclic graph obtained by attaching l_1 paths of length n_1, l_2 paths of length n_2, ..., l_m paths of length n_k, respectively, to one vertices of C_k, where $n_1 > n_2 > \cdots > n_m$. Below we characterize the extremal sparse graphs of order n and the size m with respect to the Merrifield–Simmons index where $m \in \{n-1, n, n+1\}$.

Lemma 2.2. ([4, 5, 23]) *Let G be a connected graph of order $n > 3$ with m edges.*

(i) If $m = n - 1$*, then* $F_{n+2} = i(P_n) \le i(G) \le i(S_n) = 2^{n-1} + 1$ *with left (resp. right) equality holding if and only if* $G \cong P_n$ *(resp.* $G \cong S_n$*);*

(ii) If $m = n$*, then* $F_{n+1} + F_{n-1} \le i(G) \le 3 \cdot 2^{n-3} + 1$ *with left (resp. right) equality holding if and only if* $G \cong C_3(1^{n-3})$ *or* $G \cong C_n$ *(resp.* $G \cong C_3((n-3)^1)$*);*

(*iii*) *If* $m = n+1$, *then* $i(G) \geq 5F_{n-2}$ *with equality holding if and only if* $G \cong B_n^*$ *where* B_n^* *is a graph consisting of two triangles that are connected by a path of length* $n-5$.

Proposition 2.3. *Let* F_n *be nth Fibonacci number. Then* $F_{n+2} > \binom{n+1}{3}$ *for* $n \geq 11$.

Proof. We prove the result by induction on n. For the initial cases $n \in \{11, 12\}$, we have $F_{n+2} > \binom{n+1}{3}$. The result holds trivially. Next we assume that $n \geq 13$ and the result holds for all positive integers fewer than n. Then, by the induction, we have

$$\begin{aligned} F_{n+2} = F_{n+1} + F_n &> \binom{n}{3} + \binom{n-1}{3} \\ &= \frac{(n-1)(n-2)(2n-3)}{6} > \binom{n+1}{3} . \end{aligned}$$

Note that the last inequality holds since $n^2 - 8n + 6 > 0$ when $n \geq 13$. This completes the proof of the result. ■

Lemma 2.4. ([8,10,11,25,32]) *Let* G *be a connected graph of order* $n > 3$ *with* m *edges.*

(*i*) *If* $m = n-1$, *then* $(n-1)^2 \leq W(G) \leq \binom{n+1}{3}$ *with left (resp. right) equality holding if and only if* $G \cong S_n$ *(resp.* $G \cong P_n$*);*

(*ii*) *If* $m = n$, *then* $n^2 - 2n \leq W(G) \leq \frac{n^3-7n+12}{6}$ *with left (resp. right) equality holding if and only if* $G \cong C_3(1^{n-3})$ *(resp.* $G \cong C_3((n-3)^1)$*);*

(*iii*) *If* $m = n+1$, *then* $W(G) \leq \frac{n^3-13n+30}{6}$ *with equality holding if and only if* $G \cong B_n$ *where* B_n *is a graph obtained by inserting two edges between an isolated vertex with two vertices of degrees* 2 *in* $C_3((n-2)^1)$.

Combining Lemma 2.4 (i) with the fact that the removal of any edge will increase the value of Wiener index of a connected graph, we arrive at the following result.

Lemma 2.5. ([7]) *For any connected graph* G *with* $n(G) \geq 3$, *we have* $W(G) \leq \binom{n+1}{3}$ *with equality holding if and only if* $G \cong P_n$.

Lemma 2.6. ([28]) *For any graph* G_k *with* $k \in [t]$, *we have*

$$i(G_1 \oplus G_2 \oplus \cdots \oplus G_t) = \sum_{k=1}^{t} i(G_k) - t + 1 \ .$$

3 Sparse graphs and graphs with diameter 2

In this section we focus on the comparison results between i and W for the sparse graphs and the graphs with diameter 2. First we deal with the sparse graphs in the following theorem.

Theorem 3.1. *Let G be a connected graph of order $n \geq 11$ with m edges. Then we have $i(G) > W(G)$ for $m \in \{n-1, n, n+1\}$.*

Proof. For $m = n-1$, by Lemmas 2.4 (i), 2.2 (i) and Proposition 2.3, we have

$$i(G) \geq i(P_n) = F_{n+2} > \binom{n+1}{3} = W(P_n) \geq W(G)$$

for any graph G of order $n \geq 11$ with m edges. For any graph G of order $n \geq 11$ with $m = n$ edges, by Lemmas 2.4 (ii), 2.2 (ii) and Proposition 2.3, we have

$$i(G) \geq F_{n+1} + F_{n-1} > \binom{n}{3} + \binom{n-2}{3} = \frac{n^3 - 6n^2 + 14n - 12}{3} > \frac{n^3 - 7n + 12}{6} \geq W(G).$$

For the case $m = n+1$ and $n \geq 11$, based on Lemmas 2.4 (iii), 2.2 (iii) and Proposition 2.3, we have

$$i(G) \geq 5F_{n-2} > 5\binom{n-3}{3} = \frac{5(n^3 - 12n^2 + 47n - 60)}{6} > \frac{n^3 - 13n + 30}{6} \geq W(G),$$

completing the proof. ■

From Theorem 3.1, the following result is obvious, which extends the result of trees [15] into the cases with $n - 1 \leq m \leq n + 1$.

Corollary 3.2. *Let G be a connected graph of order $n \geq 11$ with m edges. Then we have $i(G) > PW(G)$ for $m \in \{n-1, n, n+1\}$.*

Clearly, we have $W(K_n) = \binom{n}{2} > n + 1 = i(K_n)$ for any $n \geq 4$. In the following we consider the graphs with diameter at least 2. Denote by $\mathcal{G}_n^2$ the set of graphs of order $n \geq 3$ with diameter 2.

Lemma 3.3. ([34]) *Let G be a connected graph with diameter d and a connected complement.*

(i) If $d > 3$, then $\overline{G}$ has diameter $\overline{d} = 2$;

(ii) If $d = 3$, then $\overline{G}$ has a spanning subgraph which is a double star.

Lemma 3.4. ([2]) *Let G be a 2-self-centered graph of order $n \geq 5$ and with m edges. Then $m \geq 2n - 5$.*

Lemma 3.5. ([30]) *If $G \in \mathcal{G}_n^2$ has m edges, then $W(G) = n(n-1) - m$.*

Theorem 3.6. *Let G be a connected graph of order $n \geq 8$ with $m \leq n+2$ edges and a connected complement. Then $W(\overline{G}) > i(\overline{G})$.*

Proof. Since G is connected, we have $n - 1 \leq m \leq n + 2$. Note that there exists a bijection between $E(G)$ and the set of all 2-independent sets in $\overline{G}$. Moreover, there is at most a maximum clique K_4 in G since $m \leq n + 2$, which implies that $i(\overline{G}, 3) \leq 4$, $i(\overline{G}, 4) \leq 1$ and $i(\overline{G}, k) = 0$ for any $k \geq 5$. Then

$$i(\overline{G}) \leq 1 + n + m + 4 + 1 \leq 2n + 8 .$$

Note that $\overline{G}$ is connected with radius $r \geq 2$. Let d be the diameter of G. Combining the assumption $m \leq n+2$ where $n \geq 8$ with Lemma 3.4, we have $d \geq 3$. If $d = 3$, by Lemma 3.3, we have

$$W(\overline{G}) \geq \binom{n}{2} - m + 2 \times 2 + 3 \geq \binom{n}{2} - (n+2) + 7 = \frac{n(n-3)}{2} + 5 .$$

Then $W(\overline{G}) - i(\overline{G}) \geq \frac{(n-8)(n+1)}{2} + 1 > 0$. While $d > 3$, in view of Lemmas 3.3 and 3.5, we have

$$W(\overline{G}) = \binom{n}{2} + m \geq \binom{n}{2} + n - 1 = \frac{(n+2)(n-1)}{2} ,$$

which implies that $W(\overline{G}) - i(\overline{G}) \geq \frac{n(n-3)-18}{2} > 0$ for $n \geq 8$, completing the proof of the theorem. ∎

Denote by $K_{n_1,n_2,\cdots,n_t}$ the complete t-partite graph whose partition sets are of size $n_1, n_2, \cdots, n_t$, respectively, where $n_1 \leq n_2 \leq \cdots \leq n_t$. If n_i appears $k_i > 1$ times in $K_{n_1,n_2,\cdots,n_t}$, then we write as $n_i^{(k_i)}$ in it. The *generalized cocktail party graph* [29] $GCP(n, k)$ of order n is a graph obtained from K_n by deleting k independent edges with $k \leq \frac{n}{2}$, that is, $GCP(n, k) = K_{2^{(k)},1^{(n-2k)}}$. In particular, $GCP(n, \frac{n}{2})$ is just the ordinary *cocktail party graph* with $GCP(n, \frac{n}{2}) = K_{2^{(\frac{n}{2})}}$.

Lemma 3.7. *Let $G = K_{n_1,n_2,\cdots,n_t}$ be a complete t-partite graph of order n. Then we have $i(G) - W(G) = \frac{1}{2}\sum_{i=1}^{t}\left[2^{k_i+1} - (k_i - 1)^2 - 1\right] - \frac{n^2}{2} + 1$.*

Proof. Note that $G \in \mathcal{G}_n^2$ with $n = \sum_{i=1}^{t} k_i$. Then

$$m(G) = \frac{1}{2}\sum_{i=1}^{t} k_i(n-k_i) = \frac{1}{2}\Big(n^2 - \sum_{i=1}^{t} k_i^2\Big).$$

By Lemma 3.5, we have $W(G) = n(n-1) - \frac{1}{2}\Big(n^2 - \sum_{i=1}^{t} k_i^2\Big)$. Combining the fact that $K_{n_1,n_2,\cdots,n_t} = \overline{K_{n_1}} \oplus \overline{K_{n_2}} \oplus \cdots \oplus \overline{K_{n_2}}$ with Lemma 2.6, we have $i(G) = \sum_{i=1}^{t} 2^{k_i} - t + 1$. Then our result holds from some elementary calculations. ■

Theorem 3.8. *Let $G = K_{n_1,n_2,\cdots,n_t}$ be a complete t-partite graph of order $n \geq 8$. If $n_t \leq 4$, then $W(G) > i(G)$.*

Proof. Observe that $2^{x+1} \leq \sum_{k=0}^{2} \binom{x+1}{k} + \sum_{k=x-1}^{x+1} \binom{x+1}{k} = x^2 + 3x + 4$ for any positive integer $x \leq 4$. Combining this fact with Lemma 3.7, we have

$$\begin{aligned} W(G) - i(G) &= \frac{n^2}{2} - 1 + \frac{1}{2}\sum_{i=1}^{t}\Big[(k_i-1)^2 + 1 - 2^{k_i+1}\Big] \\ &\geq \frac{n^2}{2} - 1 - \frac{1}{2}\sum_{i=1}^{t}(5k_i+2) = \frac{n^2-7n}{2} + n - t - 1 > 0, \end{aligned}$$

completing the proof. ■

From Theorem 3.8, we get $W(G) > i(G)$ for any graph $G \in \{GCP(n,k) : 1 \leq k \leq \frac{n}{2}\}$. The *friendship graph* FG_n of odd order $n \geq 5$ is a graph obtained from a star S_n by inserting $\frac{n-1}{2}$ independent edges among all leaves of S_n. The *fan graph* of order n is $FA_n = K_1 \oplus P_{n-1}$ and the *wheel graph* of order n is $W_n = K_1 \oplus C_{n-1}$.

Based on Lemmas 2.1, 3.5 and Proposition 2.3, we have the following comparison result for the graphs from $\mathcal{G}_n^2$.

Proposition 3.9. $i(G) > W(G)$ *for any graph* $G \in \{FA_n, W_n : n \geq 10\} \cup \{FG_n : n \geq 9\}$.

For convenience, we set $\binom{n}{m} = 0$ if $m > n$. Next we provide a method for constructing more graphs $G \in \mathcal{G}_n^2$ with $W(G) > i(G)$.

Theorem 3.10. *Let $G_0 \in \mathcal{G}_{n_0}^2$ with $W(G_0) > i(G_0)$ and $G = K_x \oplus G_0$. Then we have $W(G) > i(G)$.*

Proof. Let $m(G_0) = m_0$. Since $G_0 \in \mathcal{G}^2_{n_0}$, then, by Lemma 3.5, we have $W(G_0) = n_0(n_0 - 1) - m_0$. By the structure of graph G, we have $i(G) = i(G_0) + x$. Note that $G \in \mathcal{G}^2_{n_0+x}$ with $m(G) = m_0 + xn_0 + \binom{x}{2}$. From Lemma 3.5, it follows that

$$\begin{aligned} W(G) &= (n_0 + x)(n_0 + x - 1) - m(G) \\ &= (n_0 + x)(n_0 + x - 1) - xn_0 - m_0 - \binom{x}{2}. \end{aligned}$$

Then we have

$$\begin{aligned} W(G) - W(G_0) &= (n_0 + x)(n_0 + x - 1) - xn_0 - m_0 - \binom{x}{2} \\ &\quad -[n_0(n_0 - 1) - m_0] \\ &= (n_0 + x)(n_0 + x - 1) - n_0(n_0 - 1) - xn_0 - \binom{x}{2} \\ &= xn_0 + \binom{x}{2}. \end{aligned}$$

Therefore we have $W(G) - i(G) > \binom{x}{2} + x(n_0 - 1) > 0$. ∎

4 Cartesian products

In this section we will present some relations between i and W in terms of Cartesian products of graphs. Below we present the formula of Wiener index of Cartesian products of two graphs.

Lemma 4.1. ([12]) *Let G and H be two connected graphs. Then*

$$W(G \,\square\, H) = n(H)^2 W(G) + n(G)^2 W(H).$$

Next, we firstly consider the Cartesian product $G \,\square\, P_2$ for any connected graph G. Note that $G \,\square\, P_2$ is also called the *prism* [24] of graph G. From the structure of $G \,\square\, P_2$, in the several results below we always assume that $V(G \,\square\, P_2) = V(G) \cup V(G')$ where $G' \cong G$ and $vv' \in E(G \,\square\, P_2)$ where $v \in V(G)$ and $v' \in V(G')$ is the corresponding vertex to v.

Lemma 4.2. *Let G be a connected graph with $n(G) = n \geq 2$. Then we have*

$$i(G \,\square\, P_2) \geq 2i(G) + n(n - 1) - 1$$

with equality holding if and only if $G \cong K_n$.

Proof. Note that any vertex $v \in V(G)$ and any different vertex in $V(G')$ from corresponding vertex to it form a 2-independent set in $G \,\square\, P_2$. Then $i(G \,\square\, P_2, 2) = n(n-1)$. So the result holds with equality holding if and only if $\alpha(G) = 1$, that is, $G \cong K_n$, completing the proof. ■

By Lemmas 4.1 and 4.2, we have $W(K_n \,\square\, P_2) = 4W(K_n) + n^2 = 3n^2 - 2n$ and $i(K_n \,\square\, P_2) = 2(n+1) - 1 + n(n-1) = n^2 + n + 1$. Therefore $W(K_n \,\square\, P_2) > i(K_n \,\square\, P_2)$. We only need to consider the Cartesian products of non-complete graphs with P_2. For two positive integers $n_1 \le n_2$, we denote by BC_{n_1,n_2} a graph obtained by connecting an isolated vertex with any vertices from complete graphs K_{n_1} and K_{n_2}, respectively, that is, $BC_{n_1,n_2} \cong K_1 \oplus (K_{n_1} \cup K_{n_2})$. Clearly, $BC_{n_1,n_2} \in \mathcal{G}^2_{n_1+n_2+1}$. Note that $BC_{1,1} = P_3$ with $i(BC_{1,1}) = 5 > 4 = W(BC_{1,1})$. In the following we focus on the comparison between i and W for the graphs BC_{n_1,n_2} and its Cartesian products with P_2.

Proposition 4.3. *Let $G = BC_{n_1,n_2}$ defined as above. Then we have $W(G) > i(G)$ for $n_1 + n_2 \ge 3$. Moreover, we have $W(G \,\square\, P_2) > i(G \,\square\, P_2)$ if and only if $n_1 = 1$ or $(n_1, n_2) \in \{(2,2),(2,3)\}$.*

Proof. Note that BC_{n_1,n_2} has diameter 2. In view of Lemma 3.5, we have

$$W(G) = (n_1+n_2+1)(n_1+n_2) - \binom{n_1}{2} - \binom{n_2}{2} - n_1 - n_2 = \binom{n_1+n_2+1}{2} + n_1 n_2 \,.$$

By Lemma 2.1 (ii), we have $i(G) = n_1 n_2 + n_1 + n_2 + 2$. It follows that

$$W(G) - i(G) = \frac{(n_1+n_2)^2}{2} - \frac{n_1+n_2}{2} - 2 = \binom{n_1+n_2}{2} - 2 > 0 \,.$$

Next we consider the graph $G \,\square\, P_2$. Note that $\alpha(G \,\square\, P_2) = 4$. From the structure of $G \,\square\, P_2$, we have $i(G \,\square\, P_2, 2) = (n_1+n_2+1)(n_1+n_2)$, $i(G \,\square\, P_2, 3) = 2n_1n_2(n_1+n_2-1)$ and $i(G \,\square\, P_2, 4) = n_1n_2(n_1-1)(n_2-1)$. Therefore we have

$$\begin{aligned} i(G \,\square\, P_2) &= 2i(G) - 1 + (n_1+n_2+1)(n_1+n_2) + 2n_1n_2(n_1+n_2-1) \\ &\quad + n_1n_2(n_1-1)(n_2-1) \\ &= (n_1+n_2+3)(n_1+n_2) + (n_1n_2+1)^2 + n_1n_2(n_1+n_2-1) + 2 \,. \end{aligned}$$

Let $\Delta = W(G\,\square\,P_2) - i(G\,\square\,P_2)$. From Lemma 4.1, it follows that

$$\begin{aligned}\Delta &= 4W(G) + (n_1+n_2+1)^2 - (n_1+n_2+3)(n_1+n_2)\\ &\quad -(n_1n_2+1)^2 - n_1n_2(n_1+n_2-1) - 2\\ &= (n_1+n_2)(2n_1+2n_2-n_1n_2+1) - n_1n_2(n_1n_2-3) - 2\\ &= (n_1+n_2)(2n_1+2n_2+1) - n_1n_2(n_1+1)(n_2+1) + 4n_1n_2 - 2\,. \qquad (1)\end{aligned}$$

From Equality (1) and some elementary calculations, our comparison result between $i(G\,\square\,P_2)$ and $W(G\,\square\,P_2)$ follows immediately. ■

Theorem 4.4. *Let G be a connected graph with $\alpha(G) \geq \frac{n(G)}{2} \geq 27$. Then we have $i(G\,\square\,P_2) > W(G\,\square\,P_2)$.*

Proof. Let $n(G) = n$ and $\alpha(G) = \alpha$. Then $\alpha \geq \frac{n}{2}$ with $n \geq 54$. Let S be a maximum independent set in G, that is, $|S| = \alpha$. Then $i(G) \geq n + 1 + \sum_{k=2}^{\alpha}\binom{\alpha}{k}$. From the structure of $G\,\square\,P_2$, any $k \geq 2$ vertices $v_1, v_2, \ldots, v_k$ from S of G and any vertex in G' not corresponding to any vertex in $\{v_1, v_2, \ldots, v_k\}$ induce a $(k+1)$-independent set in $G\,\square\,P_2$. Then

$$\begin{aligned}i(G\,\square\,P_2) &\geq 2i(G) - 1 + n(n-1) + \sum_{k=2}^{\alpha}\binom{\alpha}{k}(n-k)\\ &\geq 2\left(n+1+\sum_{k=2}^{\alpha}\binom{\alpha}{k}\right) + (n-\alpha)\sum_{k=2}^{\alpha}\binom{\alpha}{k} + n(n-1) - 1\\ &= n^2 + n + 1 + (n-\alpha+2)(2^{\alpha}-\alpha-1)\,. \qquad (2)\end{aligned}$$

Define a function $f(x) = (n-x+2)(2^x - x - 1)$ with $1 \leq x \leq n-1$. Take the differential of $f(x)$, we have $f'(x) = 2^x[(n-x)ln2 + ln4 - 1] + 2x - 1 - n > 0$ for any $x \geq \frac{n}{2}$, that is, $f(x)$ is strictly increasing for $1 \leq x \leq n-1$. Note that

$$2^{\alpha} - \alpha - 1 = \sum_{k=2}^{\alpha}\binom{\alpha}{k} > \binom{\alpha}{2} + \binom{\alpha}{3} + \binom{\alpha}{\alpha-2} + \binom{\alpha}{\alpha-1} = \frac{\alpha(\alpha+1)(\alpha+2)}{6}\,.$$

Combining Inequality (2), Lemma 4.1 with the assumption $\alpha \geq \frac{n}{2}$, we have

$$\begin{aligned}i(G\,\square\,P_2) - W(G\,\square\,P_2) &> n^2 + n + 1 + \frac{n+4}{2}\frac{n(n+2)(n+4)}{48} - n^2 - 4W(G)\\ &\geq n + 1 + \frac{n(n+2)(n+4)^2}{96} - \frac{2n(n^2-1)}{3}\\ &> \frac{(n+2)(n+4)^2 + 96 - 64(n^2-1)}{96}\\ &= \frac{n^2(n-54) + 32n + 192}{96} > 0\end{aligned}$$

for any $n \geq 54$. This completes the proof of the theorem. ■

Let $\beta(G)$ be the matching number of a graph G. Note that [1] $\alpha(G) + \beta(G) = n$ for any connected bipartite graph G of order n. Since $\beta(G) \leq \lfloor \frac{n}{2} \rfloor$ for any connected bipartite graph G of order $n \geq 2$, we have $\alpha(G) \geq \lceil \frac{n}{2} \rceil$. From Theorem 4.4, we deduce the following result.

Corollary 4.5. *Let G be a connected bipartite graph of order $n \geq 54$. Then we have $i(G \,\square\, P_2) > W(G \,\square\, P_2)$.*

Below we prove a stronger result on the comparison result between i and W for the Cartesian products of graphs with stars S_n.

Theorem 4.6. *Let G be a connected graph. Then $i(G \,\square\, S_n) > W(G \,\square\, S_n)$ for any integer $n \geq 6$.*

Proof. Note that $i(G) \geq n(G) + 1$. Let $V(S_n) = \{v_1, v_2, \ldots, v_n\}$ with v_1 as its center. From the structure of $G \,\square\, S_n$, $V(G \,\square\, S_n)$ can be partitioned as $V(G_1) \cup V(G_2) \cup \cdots \cup V(G_n)$ with $V(G_i) = \{v_i\} \times V(G)$ for $i \in [n]$. Then the set of vertices from k distinct graphs from $\bigcup_{p=2}^{n} G_p$ is just a k-independent set in $G \,\square\, S_n$ for $k \in [n] \setminus \{1\}$. Thus we have

$$\begin{aligned}
i(G \,\square\, S_n) &\geq ni(G) - (n-1) + (n-1)n(G)[n(G)-1] + \binom{n-1}{2} n(G)^2 \\
&\quad + \binom{n-1}{3} n(G)^3 + \sum_{k=0}^{3} \binom{n-1}{n-1-k} n(G)^{n-1-k} \\
&> \left[\binom{n}{2} + \binom{n-1}{n-4}\right] n(G)^2 + \binom{n-1}{3} n(G)^3 + \sum_{k=0}^{2} \binom{n-1}{n-1-k} n(G)^{n-1-k} \\
&> \frac{(n-1)(n^2-2n+6)}{6} n(G)^2 + \left[\binom{n}{3} + n\right] n(G)^3 ,
\end{aligned}$$

for any $n \geq 6$. By Lemmas 2.5, 4.1, we have

$$\begin{aligned}
i(G \,\square\, S_n) - W(G \,\square\, S_n) &> \frac{(n-1)(n^2-2n+6)}{6} n(G)^2 + \frac{n(n^2-3n+8)}{6} n(G)^3 \\
&- (n-1)^2 n(G)^2 - n^2 W(G) \\
&\geq \frac{(n-1)(n-2)(n-6)}{6} n(G)^2 + \frac{n(n^2-3n+8)}{6} n(G)^3 \\
&- n^2 \binom{n(G)+1}{3} > \frac{n(n^2-4n+8)}{6} n(G)^3 > 0 ,
\end{aligned}$$

completing the proof. ■

5 Concluding remarks

In this paper we report some relations between $i(G)$ and $W(G)$ for connected graphs G, including sparse graphs of order n with m $(n-1 \leq m \leq n+1)$ edges and their complements, as well as for some graphs with diameter 2. Moreover, some relations between these two invariants are established in terms of Cartesian products of graphs, especially $G \,\square\, P_2$ and $G \,\square\, S_n$.

By some elementary calculations, we get $i(S_4) = W(S_4) = 9$. But, except S_4, do there exist other graphs with $i(G) = W(G)$? Furthermore, determining all connected graphs with $i(G) = W(G)$ seems an unknown but challenging problem to us.

In Section 3, we provide some sufficient conditions of $W(G) > i(G)$ (resp. $i(G) > WG)$) for the graphs G with diameter 2. Here we propose the following problem for the graphs with diameter 2.

Problem 5.1. *How to characterize all the graphs G with diameter 2 satisfying different comparison results between $i(G)$ and $W(G)$?*

Recall that $i(BC_{1,1}) = 5 > 4 = W(BC_{1,1})$ with $i(P_2) > W(P_2)$. But, by Proposition 4.3, we have $W(BC_{1,1} \,\square\, P_2) > i(BC_{1,1} \,\square\, P_2)$. Moreover, although from Proposition 4.3 $W(BC_{n_1,n_2}) > i(BC_{n_1,n_2})$ holds for any n_1, n_2 with $n_1 + n_2 \geq 3$, we have

$$W(BC_{n_1,n_2} \,\square\, P_2) - i(BC_{n_1,n_2} \,\square\, P_2) = \begin{cases} 5, & (n_1, n_2) = (2, 3); \\ -12, & (n_1, n_2) = (2, 4). \end{cases}$$

Based on the above fact, we would like to pose the following problem.

Problem 5.2. *How to characterize the Cartesian products G of graphs $G \,\square\, H$ and H with hereditary comparison property with respect to i and W, that is, $i(G \,\square\, H) \gtrless W(G \,\square\, H)$ for graph G and H with $i(G) \gtrless W(H)$ and $i(H) \gtrless W(H)$?*

From Theorem 3.1, we find that $i(G) > W(G)$ for some sparse connected graphs G of order $n \geq 11$ with m edges when $n-1 \leq m \leq n+1$. Now we would like to end this paper with the following relevant problem.

Problem 5.3. *Can we find a constant $c(n)$ such that $i(G) > W(G)$ for any connected graphs G with $n(G) = n$ and m edges where $m \leq c(n)$?*

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