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On the Merrifield–Simmons Index of Graphs *

Haixing Zhao Ruying Liu

Department of Mathematics
Qinghai Normal University
Xining, Qinghai 810008, P.R. China

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Abstract

Let G be a (molecular) graph G. The Merrifield and Simmons index of G, denoted by $\sigma(G)$, is defined as the number of subsets of the vertex set $V(G)$ in which no two vertices are adjacent in G, i.e., the number of independent sets of G. In this paper, we determine all connected graphs G with $2^{n-2} \leq \sigma(G) \leq 2^{n-1}$, for $n \geq 10$. As a byproduct, the graphs of n vertices and m edges with the largest, the second largest Merrifield and Simmons index are obtained, for $n \leq m \leq 2n-3$.

1 Introduction

All graphs considered here are finite and simple. Undefined notations and terminology will conform to those in [2].

For a molecular graph G, the Merrifield and Simmons index $\sigma(G)$, or simply σ-index, is defined as the number of subsets of $V(G)$ in which no two vertices are adjacent in G, i.e., in graph-theoretical terminology, the number of independent sets of G, including the empty set. For example, for the circle of 4 vertices $C_4 = v_1v_2v_3v_4$, all such subsets of $V(C_4)$ are as follows: ϕ, $\{v_1\}$, $\{v_2\}$, $\{v_3\}$, $\{v_4\}$, $\{v_1, v_3\}$, $\{v_2, v_4\}$, and so $\sigma(C_4) = 7$. In monograph [11], Merrifield and Simmons showed that the σ-index of a molecular graph is correlated with its boiling points. The σ-index of a molecular graph was extensively studied in [3-15].

For a graph G, we denote by $V(G)$ the vertex set of G and by $E(G)$ the edge set of G. Let $u \in V(G)$, by $N_G(u)$ we denote the set of all neighbors of u in G. For two graphs G and H, we denote by $G \cup H$ the disjoint union of G and H and by mH the disjoint union of m copies of H. We denote by P_n, S_n and C_n the path, the star, the circle of n vertices, respectively. Denote by K_n the complete graph of n vertices. For a graph G, $\overline{G}$ denotes the complement of G.

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For the path P_n, $\sigma(P_n)$ is exactly the famous Fibonacci number F_{n+2} such that $F_n = F_{n-1} + F_{n-2}$ with initial conditions $F_0 = 0$ and $F_1 = 1$. In 1984, Prodinger and Tichy [13] proved that every tree T on n vertices satisfies $F_{n+2} \leq \sigma(T) \leq 2^{n-1} + 1$. In [9], the authors characterized all trees T with $2^{n-2} \leq \sigma(T) \leq 2^{n-1}$. Very recently, Pedersen and Vestergaard [12] gave the lower bound and the upper bound of $\sigma(G)$ for unicyclic graphs.

In this paper, we shall investigate the σ-index for all connected graphs. We characterize all connected graphs with σ-index between 2^{n-2} and 2^{n-1}, for $n \geq 10$. As a byproduct, we also give the graphs of n vertices and m edges with the largest, the second largest σ-index, where $n \leq m \leq 2n-3$.

2 Some Lemmas

Let T be a tree with n vertices. Denote by $\mathcal{T}(n)$ the set of trees with n vertices. From [1, 8, 12, 13], we can find the following results.

Lemma 1.([8, 13]) Let T be a tree with n vertices. Then $F_{n+2} \leq \sigma(T) \leq 2^{n-1} + 1$ and $\sigma(T) = F_{n+2}$ if and only if $T \cong P_n$ and $\sigma(T) = 2^{n-1} + 1$ if and only if $T \cong S_n$.

Lemma 2. ([8, 13]) Let G be a graph with k components $G_1, G_2, \cdots, G_k$. Then

$$\sigma(G) = \prod_{i=1}^{k} \sigma(G_i).$$

Lemma 3. ([8]) For a graph G with $v \in V(G)$, we have

$$\sigma(G) = \sigma(G - v) + \sigma(G - [v]),$$

where $[v] = N_G(v) \cup \{v\}$.

Lemma 4. ([12]) For a graph G with $vu \in V(G)$, we have

$$\sigma(G) = \sigma(G - uv) - \sigma(G - N[uv]),$$

where $N[uv] = N_G(v) \cup N_G(u)$.

Lemma 5. ([1]) Let G_1 and G_2 be two graphs. If $V(G_1) = V(G_2)$ and $E(G_1) \subset E(G_2)$, then $\sigma(G_1) > \sigma(G_2)$.

3 Graphs G of n vertices with $2^{n-2} \leq \sigma(G) \leq 2^{n-1}$

The graphs shown in Figures 1 and 2 are frequently used throughout the paper. The graphs used in Theorems 2 and 3 are shown in Figures 3, 4 and 5.

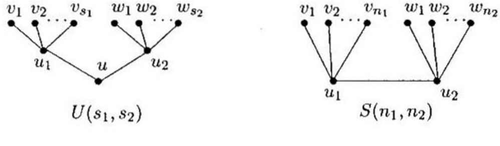

Figure 1. Graphs $U(s_1, s_2)$ and $S(n_1, n_2)$ with $s_1 + s_2 = n - 3$ and $n_1 + n_2 = n - 2$.

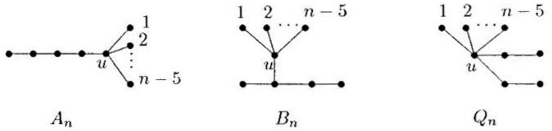

Figure 2. Graphs A_n, B_n and Q_n

In [9], the authors determined the all trees T with $2^{n-2} \leq \sigma(T) \leq 2^{n-1}$ as follows:

Theorem 1. ([9]) If $T \in \mathcal{T}(n)$ and $n \geq 10$, then $2^{n-2} \leq \sigma(T) \leq 2^{n-1}$ if and only if $T \in \{A_n, B_n, Q_n, U(s_1, s_2), S(n_1, n_2) | n_1 + n_2 = n-2, 1 \leq n_1 \leq n_2, s_1 + s_2 = n-3, 1 \leq s_1 \leq s_2\}$. In addition, $\sigma(A_n) = 2^{n-2} + 5$, $\sigma(B_n) = 2^{n-2} + 6$, $\sigma(Q_n) = 2^{n-2} + 2^{n-5} + 4$, $\sigma(U(s_1, s_2)) = 2^{n-2} + 2^{s_1} + 2^{s_2} + 1$, $\sigma(S(n_1, n_2)) = 2^{n-2} + 2^{n_1} + 2^{n_2}$.

In this paper, we get the following theorem.

Theorem 2. Let $n \geq 10$ and let G be a connected graph of n vertices with $G \notin \mathcal{T}(n)$. Then $2^{n-2} \leq \sigma(G) \leq 2^{n-1}$ if and only if $G \in \{A_{n,i} | i = 1,2,3,4,5,6,7,8,9\} \cup \{B_{n,i} | i = 1,2,3\} \cup \{U(t_1, t_2, t_3) | 0 \leq t_1 \leq t_3, 1 \leq t_2, t_1 + t_2 + t_3 = n-3\} \cup \{S(l_1, l_2, l_3) | 0 \leq l_1 \leq l_3, 1 \leq l_2, l_1 + l_2 + l_3 = n-2\}$. In addition, $\sigma(A_{n,1}) = \sigma(A_{n,3}) = \sigma(B_{n,1}) = 2^{n-2} + 3$, $\sigma(A_{n,2}) = \sigma(A_{n,7}) = 2^{n-2} + 4$, $\sigma(A_{n,4}) = \sigma(A_{n,5}) = \sigma(B_{n,2}) = 2^{n-2} + 2$, $\sigma(A_{n,6}) = \sigma(B_{n,3}) = 2^{n-2} + 1$, $\sigma(A_{n,8}) = 2^{n-2} + 2^{n-5} + 2$, $\sigma(A_{n,9}) = 2^{n-2} + 2^{n-5} + 1$, $\sigma(U(t_1, t_2, t_3)) = 2^{n-2} + 2^{t_1} + 2^{t_3} + 1$, $\sigma(S(l_1, l_2, l_3)) = 2^{n-2} + 2^{l_1} + 2^{l_3}$.

From Theorem 2, it follows that

Theorem 3. Let $n \geq 10$ and let G be a connected graph of n vertices with $G \notin \mathcal{T}(n)$. Then we have

(i) for $m = 2n-3$, the unique graph with the largest Merrifield-Simmons index is $S(0, n-2, 0)$, where $\sigma(S(0, n-2, 0)) = 2^{n-2} + 2$,

(ii) for $m = 2n-4$, the graphs with the largest Merrifield-Simmons index are $S(0, n-3, 1)$ and $U(0, n-3, 0)$, where $\sigma(S(0, n-3, 1)) = \sigma(U(0, n-3, 0)) = 2^{n-2} + 3$,

(iii) for $m = 2n-k-3$, where $2 \leq k \leq n-3$, the unique graph with the largest Merrifield-Simmons index is $S(0, n-k-2, k)$ and the graphs with second largest Merrifield-Simmons index are $S(1, n-k-2, k-1)$ and $U(0, n-k-2, k-1)$, where $\sigma(S(0, n-k-2, k)) = 2^{n-2} + 2^k + 1$ and $\sigma(S(1, n-k-2, k-1)) = \sigma(U(0, n-k-2, k-1)) = 2^{n-2} + 2^{k-1} + 2$. □

4 The Proof of Theorem 2

Lemma 6. Let $n \geq 10$ and let G be a graph of n vertices with $u \in V(G)$ and $\sigma(G - [u]) \leq 2^3$. Then $2^{n-2} \leq \sigma(G) \leq 2^{n-1}$ if and only if $G - u \in \{C_3 \cup (n-4)K_1, P_4 \cup (n-5)K_1, S_r \cup (n-r-1)K_1, 2P_2 \cup (n-5)K_1 | r \geq 2\}$.

Proof. If $G - u \in \{C_3 \cup (n-4)K_1, P_4 \cup (n-5)K_1, S_r \cup (n-r-1)K_1, 2P_2 \cup (n-5)K_1 | r \geq 2\}$, by Lemma 2 it is easy to see that $2^{n-2} \leq \sigma(G-u) \leq 2^{n-2} + 2^{n-r-1}$, for $n \geq 10$. From Lemma 3, $2^{n-2} < \sigma(G) \leq 2^{n-1}$. Otherwise, $G - u$ must contain one of the following graphs as its spanning subgraphs:

$$G' \in \{P_5 \cup (n-6)K_1, C_4 \cup (n-5)K_1, D_4 \cup (n-5)K_1,$$

$$P_2 \cup P_3 \cup (n-6)K_1, 3P_2 \cup (n-7)K_1\},$$

where D_4 denotes the graph obtained from C_3 by adding a pendant edge. For $n \geq 10$, it is easy to verify that $\sigma(G') + 2^3 < 2^{n-2}$ for each graph G' above. By Lemmas 3 and 5, we have that

$$\sigma(G) = \sigma(G-u) + \sigma(G-[u]) \leq \sigma(G') + 2^3 < 2^{n-2}.$$

The proof is completed. □

Lemma 7. For $n \geq 10$, let G be the graph of n vertices obtained from Y by adding some edges of $\overline{Y}$ to Y, where $Y \in \{A_n, B_n, Q_n\}$. Then $2^{n-2} \leq \sigma(G) \leq 2^{n-1}$ if and only if $G \in \{A_{n,1}, A_{n,2}, A_{n,3}, A_{n,4}, A_{n,5}, A_{n,6}, A_{n,7}, A_{n,8}, A_{n,9}\}$, where $A_{n,i} (1 \leq i \leq 9)$ are as shown in Figure 3. In addition, $\sigma(A_{n,1}) = \sigma(A_{n,3}) = 2^{n-2} + 3$, $\sigma(A_{n,2}) = \sigma(A_{n,7}) = 2^{n-2} + 4$, $\sigma(A_{n,4}) = \sigma(A_{n,5}) = 2^{n-2} + 2$, $\sigma(A_{n,6}) = 2^{n-2} + 1$, $\sigma(A_{n,8}) = 2^{n-2} + 2^{n-5} + 2$, $\sigma(A_{n,9}) = 2^{n-2} + 2^{n-5} + 1$.

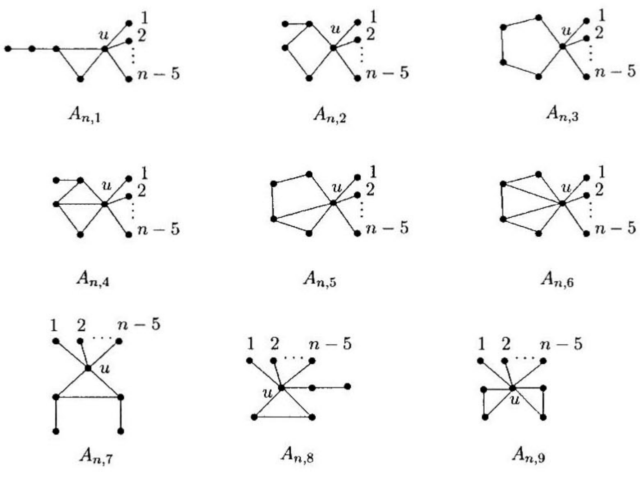

Figure 3. Graphs $A_{n,i}$, $i = 1, 2, 3, 4, 5, 6, 7, 8, 9$.

Proof. Suppose that G is the graph obtained from Y by adding some edges of $\overline{Y}$ to Y, where $Y \in \{A_n, B_n, Q_n\}$. For each Y, there exists the vertex u such that $\sigma(Y - [u]) \leq 2^3$, see Figure 2. By Lemma 5, $\sigma(G - [u]) \leq 2^3$, for each G. It follows, from Lemma 6, that $2^{n-2} \leq \sigma(G) \leq 2^{n-1}$ if and only if $G - u \in \{C_3 \cup (n-4)K_1, P_4 \cup (n-5)K_1, S_r \cup (n-r-1)K_1, 2P_2 \cup (n-5)K_1 | r \geq 2\}$. So, G is one of the graphs $A_{n,i}$ as shown in Figure 3, where $i = 1, 2, 3, 4, 5, 6, 7, 8, 9$. By Lemmas 2 and 3, it is easy to get their σ-indices. This completes the proof. □

Lemma 8. Let $n \geq 10$ and $|V(G)| = n$. Let G be the graph obtained from $U(s_1, s_2)$ by adding some edges of $\overline{U(s_1, s_2)}$ to $U(s_1, s_2)$, where $s_1 + s_2 = n - 3$. Then $2^{n-2} \leq \sigma(G) \leq 2^{n-1}$ if and only if $G \in \{A_{n,1}, A_{n,3}, A_{n,4}, A_{n,5}, A_{n,6}, B_{n,1}, B_{n,2}, B_{n,3}\} \cup \{U(t_1, t_2, t_3) | 0 \leq t_1 \leq t_3, 1 \leq t_2, t_1 + t_2 + t_3 = n - 3\} \cup \{S(l_1, l_2, l_3) | 0 \leq l_1 \leq l_3, 1 \leq l_2, l_1 + l_2 + l_3 = n - 2\}$, where $A_{n,i}$ are the graphs shown in Figure 3, $B_{n,i}$ are graphs shown in Figure 4, $U(t_1, t_2, t_3)$ and $S(l_1, l_2, l_3)$ are the graphs shown in Figure 5. In addition, $\sigma(B_{n,1}) = 2^{n-2} + 3$, $\sigma(B_{n,2}) = 2^{n-2} + 2$, $\sigma(B_{n,3}) = 2^{n-2} + 1$, $\sigma(U(t_1, t_2, t_3)) = 2^{n-2} + 2^{t_1} + 2^{t_3} + 1$, $\sigma(S(l_1, l_2, l_3)) = 2^{n-2} + 2^{l_1} + 2^{l_3}$.

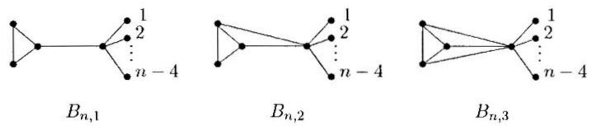

Figure 4. Graphs $B_{n,i}$, $i = 1, 2, 3$.

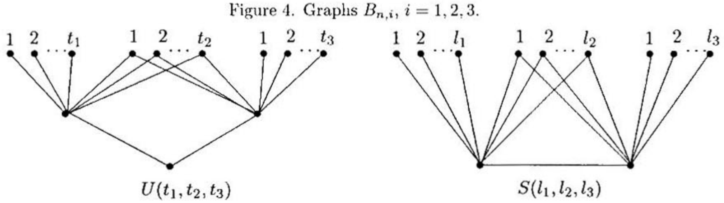

Figure 5. Graphs $U(t_1, t_2, t_3)$ and $S(l_1, l_2, l_3)$.

Proof. Denote by Ω the set of some edges in $\overline{U(s_1, s_2)}$ such that the graph G obtained from $U(s_1, s_2)$ by adding all edges in the set Ω satisfy $2^{n-2} \le \sigma(G) \le 2^{n-1}$. Write $G = U(s_1, s_2) + \Omega$. By Lemma 5, it is not hard to see that if $\Phi \subseteq \Omega$ and $\sigma(U(s_1, s_2) + \Omega) \ge 2^{n-2}$, then $\sigma(U(s_1, s_2) + \Phi) \ge \sigma(U(s_1, s_2) + \Omega) \ge 2^{n-2}$. According the construction of $U(s_1, s_2)$(see Figure 1), we consider the following cases:

Case 1. Suppose $v_1 v_2 \in \Omega$. By Lemmas 4 and 5, we have

$$\sigma(G) \le \sigma(U(s_1, s_2)) - \sigma((s_1 - 2)K_1 \cup S_{s_2+2}).$$

Note that $s_1 + s_2 = n - 3$ and $s_1 \ge 2$. It follows, by Theorem 1 and Lemma 2, that

$$\sigma(G) \le 2^{n-2} + 2^{s_1} + 2^{s_2} + 1 - 2^{n-4} - 2^{s_1-2}.$$

Since $n \ge 10$ and $n - 5 > s_1$, we have $\sigma(G) < 2^{n-2}$.

Case 2. Suppose $w_1 w_2 \in \Omega$. It follows from Theorem 1, Lemmas 2, 4 and 5 that

$$\begin{aligned} \sigma(G) &\le \sigma(U(s_1, s_2)) - \sigma((s_2 - 2)K_1 \cup S_{s_1+2}) \\ &= 2^{n-2} + 2^{s_1} + 2^{s_2} + 1 - 2^{n-4} - 2^{s_2-2}. \end{aligned}$$

Note that $s_1 + s_2 = n - 3$ and $1 \le s_1 \le s_2 \le n - 4$. If $s_1 = 1$ and $s_2 = n - 4$, then $\sigma(G) \le 2^{n-2} + 3 - 2^{n-6} < 2^{n-2}$. Otherwise $2 \le s_1 \le s_2 \le n - 5$ and $n - 5 > s_1$, for $n \ge 10$, and so $\sigma(G) < 2^{n-2}$.

Case 3. Suppose $v_1 u \in \Omega$. By Lemmas 2, 4 and 5, we have

$$\sigma(G) \le 2^{n-2} + 2^{s_1} + 2^{s_2} + 1 - 2^{n-4}.$$

Note that $s_1 + s_2 = n - 3$ and $1 \le s_1 \le s_2 \le n - 4$. We have $s_1 = 1$ and $s_2 = n - 4$. (Otherwise $2 \le s_1 \le s_2 \le n - 5$ and $n - 5 > s_1$, for $n \ge 10$, and then $\sigma(G) < 2^{n-2}$.) If $\Omega = \{v_1 u\}$, then

$\sigma(G) = 2^{n-2} + 3$ and $G \cong B_{n,1}$. Since $B_{n,1}$ contains a vertex x such that $\sigma(B_{n,1} - [x]) < 2^3$, by a argument similar with that of Lemma 7 we have that if $v_1u \in \Omega$, then $G \in \{B_{n,1}, B_{n,2}, B_{n,3}\}$.

Case 4. Suppose $w_1u \in \Omega$. By Lemmas 2, 4 and 5,

$$\sigma(G) \leq 2^{n-2} + 2^{s_1} + 2^{s_2} + 1 - 2^{n-4}.$$

Note that $s_1 + s_2 = n - 3$ and $1 \leq s_1 \leq s_2 \leq n - 4$. We have $s_1 = 1$ and $s_2 = n - 4$. (Otherwise $2 \leq s_1 \leq s_2 \leq n - 5$ and $n - 5 > s_1$, for $n \geq 10$, and then $\sigma(G) < 2^{n-2}$.) If $\Omega = \{w_1u\}$, then $\sigma(G) = 2^{n-2} + 3$ and $G \cong A_{n,1}$. For $A_{n,1}$, by a argument similar with that of Lemma 7 we know that if $w_1u \in \Omega$, then $G \in \{A_{n,1}, A_{n,4}, A_{n,5}, A_{n,6}\}$.

Case 5. Suppose $v_1w_1 \in \Omega$. By Lemmas 2, 4 and 5, we have

$$\sigma(G) \leq 2^{n-2} + 2^{s_1} + 2^{s_2} + 1 - 2^{n-4}.$$

Note that $s_1 + s_2 = n - 3$ and $1 \leq s_1 \leq s_2 \leq n - 4$. We have $s_1 = 1$ and $s_2 = n - 4$. (Otherwise $2 \leq s_1 \leq s_2 \leq n - 5$, $n - 5 > s_1$ when $n \geq 10$, and then $\sigma(G) < 2^{n-2}$.)If $\Omega = \{v_1w_1\}$, then $\sigma(G) = 2^{n-2} + 3$ and $G \cong A_{n,3}$. For $A_{n,3}$, by a argument similar with that of Lemma 7 we have that if $v_1w_1 \in \Omega$, then $G \in \{A_{n,3}, A_{n,5}, A_{n,6}\}$.

Case 6. $x \in \{u_1, u_2\}$ or $y \in \{u_1, u_2\}$ for each $xy \in \Omega$. If $u_1u_2 \in \Omega$, then all graphs are the graphs $S(l_1, l_2, l_3)$ shown in Figure 5, where $0 \leq l_1 \leq l_3$, $1 \leq l_2$ and $l_1 + l_2 + l_3 = n - 2$. Otherwise all graphs are the graphs $U(t_1, t_2, t_3)$ shown in Figure 5, where $0 \leq t_1 \leq t_3$, $1 \leq t_2$ and $t_1 + t_2 + t_3 = n - 3$. By Lemmas 2 and 3, it is easy to get that

$$\sigma(U(t_1, t_2, t_3)) = 2^{n-2} + 2^{t_1} + 2^{t_3} + 1$$

and

$$\sigma(S(l_1, l_2, l_3)) = 2^{n-2} + 2^{l_1} + 2^{l_3}.$$

From the above argument, the lemma follows. □

Lemma 9. Let $n \geq 10$ and $|V(G)| = n$. Let G be the graph obtained from $S(n_1, n_2)$ by adding some edges of $\overline{S(n_1, n_2)}$. Then $2^{n-2} \leq \sigma(G) \leq 2^{n-1}$ if and only if $G \in \{A_{n,2}, A_{n,4}, A_{n,5}, A_{n,6}, A_{n,8}, A_{n,9}, B_{n,1}, B_{n,2}, B_{n,3}\} \cup \{S(l_1, l_2, l_3) | 0 \leq l_1 \leq l_3, 1 \leq l_2, l_1 + l_2 + l_3 = n - 2\}$.

Proof. Denote by Ω' the set of some edges in $\overline{S(n_1, n_2)}$ such that the graph G obtained from $S(n_1, n_2)$ by adding all edges in the set Ω' satisfy $2^{n-2} \leq \sigma(G) \leq 2^{n-1}$. By the construction of $S(n_1, n_2)$ (see Figure 1), we distinguish the following cases:

Case 1. Suppose $v_1v_2 \in \Omega'$. By Theorem 1 and Lemmas 2, 4 and 5,

$$\sigma(G) \leq 2^{n-2} + 2^{n_1} + 2^{n_2} - 2^{n-4} - 2^{n_1-2}.$$

Note that $n \geq 10$, $n_1 + n_2 = n - 2$ and $2 \leq n_1 \leq n_2 \leq n - 4$. We have $n_1 = 2$ and $n_2 = n - 4$. (Otherwise $3 \leq n_1 \leq n_2 \leq n - 5$ and $n - 5 > n_1$, and so $\sigma(G) < 2^{n-2}$.)If $\Omega' = \{v_1v_2\}$, then $\sigma(G) = 2^{n-2} + 3$ and $G \cong B_{n,1}$. From Case 3 of the proof in Lemma 8, we have that if $v_1v_2 \in \Omega'$, then $G \in \{B_{n,1}, B_{n,2}, B_{n,3}\}$.

Case 2. Suppose $w_1w_2 \in \Omega'$. By Lemmas 2, 4 and 5,

$$\sigma(G) \leq 2^{n-2} + 2^{n_1} + 2^{n_2} - 2^{n-4} - 2^{n_2-2}.$$

Note that $n \geq 10$, $n_1 + n_2 = n - 2$ and $1 \leq n_1 \leq n_2 \leq n - 3$. We have $n_1 = 1$ and $n_2 = n - 3$. (Otherwise $2 \leq n_1 \leq n_2 \leq n - 4$, it easy to see that $\sigma(G) < 2^{n-2}$.)If $\Omega' = \{w_1w_2\}$, then $\sigma(G) = 2^{n-2} + 2^{n-5} + 2$ and $G \cong A_{n,8}$. For $A_{n,8}$, it follows, by a similar argument with that of Lemma 7, that if $w_1w_2 \in \Omega'$, then $G \in \{A_{n,4}, A_{n,5}, A_{n,6}, A_{n,8}, A_{n,9}\}$.

Case 3. Suppose $v_1w_1 \in \Omega'$. By Lemmas 2, 4 and 5, we get that

$$\sigma(G) \leq 2^{n-2} + 2^{n_1} + 2^{n_2} - 2^{n-4}.$$

Note that $n \geq 10$, $n_1 + n_2 = n - 2$ and $1 \leq n_1 \leq n_2 \leq n - 3$. We have that $n_1 = 1$ and $n_2 = n - 3$ or $n_1 = 2$ and $n_2 = n - 4$. (Otherwise $3 \leq n_1 \leq n_2 \leq n - 5$, it follows that $n - 5 > n_1$ and $\sigma(G) < 2^{n-2}$.) If $\Omega' = \{v_1w_1\}$, then $\sigma(G) = 2^{n-2} + 2^{n-4} + 2$ and $G \cong U(0, 1, n-4)$ for $n_1 = 1$ and $n_2 = n - 3$ or $\sigma(G) = 2^{n-2} + 4$ and $G \cong A_{n,2}$ for $n_1 = 2$ and $n_2 = n - 4$. With a similar argument of Lemma 7, for $A_{n,2}$ and $U(0, 1, n - 4)$, we have that if $v_1w_1 \in \Omega'$, then $G \in \{A_{n,2}, A_{n,4}, A_{n,5}, A_{n,6}, B_{n,2}, B_{n,3}\}$.

Case 4. $x \in \{u_1, u_2\}$ or $y \in \{u_1, u_2\}$ for each $xy \in \Omega'$. Then all graphs are the graphs $S(l_1, l_2, l_3)$(see Figure 5). By Lemma 8, we have

$$\sigma(S(l_1, l_2, l_3)) = 2^{n-2} + 2^{l_1} + 2^{l_3}.$$

From the above argument, the lemma holds. □

By Lemma 6 and a similar argument with that of Lemma 7, we have

Lemma 10. Let $n \geq 10$ and $|V(G)| = n$. Let G be the graph obtained from S_n by adding some edges of $\overline{S_n}$. Then $2^{n-2} \leq \sigma(G) \leq 2^{n-1}$ if and only if $G \in \{A_{n,9}, B_{n,3}\} \cup \{S(0, l_2, l_3) | 1 \leq l_2, l_2 + l_3 = n - 2\}$. □

The proof of Theorem 2: Suppose that G is a connected graph of n vertices with $2^{n-2} \leq \sigma(G) \leq 2^{n-1}$, where G is not a tree. Then G must be obtained from a tree T of n vertices by adding some edges of $\overline{T}$. By Lemma 5, we have that if $\sigma(T) < 2^{n-2}$, then $\sigma(G) \leq \sigma(T) < 2^{n-2}$. For $n \geq 10$, all graphs T with $\sigma(T) \geq 2^{n-2}$ are given by Lemma 1 and Theorem 1. Thus, the theorem follows from Lemmas 7 to 10. □

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