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CONNECTED GRAPHS WITH A LARGE NUMBER OF INDEPENDENT SETS

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Abstract. For a simple undirected graph $G = (V(G), E(G))$, a subset I of $V(G)$ is said to be an independent set of G if any two vertices in I are not adjacent in G. An empty set is also an independent set in G. The set of all independent sets of a graph G is denoted by $I(G)$ and its cardinality by $i(G)$ (known as the Merrifield-Simmons index in mathematical chemistry). Let $h(n, x)$ be the x-th largest number of independent sets among all connected n-vertex graphs. In this paper, we determine the numbers $h(n, x)$ for $1 \leq x \leq \lfloor \frac{n}{2} \rfloor^2 - 3 \cdot \lfloor \frac{n}{2} \rfloor + 3$. Besides, we also characterize the connected n-vertex graphs achieving these values.

1. Introduction and Preliminary

Given a graph $G = (V(G), E(G))$, a subset $S \subseteq V(G)$ is called *independent set* if no two vertices of S are adjacent in G. An empty set is also an independent set in G. The set of all independent sets of a graph G is denoted by $I(G)$ and its cardinality by $i(G)$. For a vertex $v \in V(G)$, let $I_{-v}(G) = \{S \in I(G) : v \notin S\}$ and $I_{+v}(G) = \{S \in I(G) : v \in S\}$. Their cardinalities are denoted by $i_{-v}(G)$ and $i_{+v}(G)$, respectively. Note that $i(G) = i_{-v}(G) + i_{+v}(G)$. The study of the number of independent sets in a graph has a long history. This number is also called the Merrifield-Simmons index. The Merrifield-Simmons index was introduced by Merrifield and Simmons [8] in 1989. In [4] Gutman first named its index the Merrifield-Simmons index. This index is one of the most popular topological indices in mathematical chemistry, there is a correlation between this index and boiling points. There are researchers developed a topological approach to structural chemistry (see [5, 8, 11]).

Enumerating independent sets in a graph is well-studied problem arising in many fields. Much recent research has focused on the problem of maximizing the number of in a special graph with certain restrictions (see [1, 3]). Several papers deal with

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the characterization of the extremal graphs with respect to this number in some special graphs. The problem was extensively studied for various classes of graphs, including trees ([6, 13]), unicyclic graphs ([1, 9]), regular bipartite graphs [2] and $(n, n+2)$-graphs [5]. It is known [10] that the star $K_{1,n-1}$ has the largest number of independent sets and the path P_n has the smallest number of independent sets among all trees with n vertices. The problems of determining the second largest and the second smallest values of independent sets for a tree T with n vertices and those graphs achieving these values were solved in [6] and [7], respectively. For $1 \le x$, let $h(n, x)$ be the x-th largest number of independent sets among all connected n-vertex graphs. In this paper, we determine the numbers $h(n, x)$ for $1 \le x \le \lfloor \frac{n}{2} \rfloor^2 - 3 \cdot \lfloor \frac{n}{2} \rfloor + 3$. Besides, we also characterize the connected n-vertex graphs achieving these values.

In order to state our results, we introduce some notation and terminology. For other undefined terms we refer to [12]. We denote by $G = (V(G), E(G))$ a graph of order $n = |G|$. The graph G is called *null* if $|G| = 0$. A maximal connected subgraph of G is called a *component* of G. For a subset $X \subseteq V(G)$, we define the *neighborhood* $N_G(X)$ of X in G to be the set of all vertices adjacent to vertices in X and the *closed neighborhood* $N_G[X] = N_G(X) \cup X$. For a vertex $x \in V(G)$, let $\deg_G(x)$ denote its *degree*. A *leaf* is a vertex of degree 1. For a subset $A \subseteq V(G)$, the *deletion of A from* G is the graph $G - A$ obtained from G by removing all vertices in A and all edges incident to these vertices. If $A = \{v\}$, we write $G-v$ instead of $G-\{v\}$. For a subset $B \subseteq E(G)$, the *edge-deletion of B from G* is the graph $G - B$ obtained from G by removing all edges in B. If $B = \{e\}$, we write $G - e$ instead of $G - \{e\}$. If a graph G is isomorphic to another graph H, we denote $G = H$. nG is the short notation for the union of n copies of disjoint graphs isomorphic to G. For $n \ge 1$, P_n a *path* with n vertices and $K_{1,n-1}$ a *star* with n vertices. Note that $K_{1,0} = P_1$. The following useful lemmas and theorems which are needed in this paper.

Lemma 1.1. ([6, 7]) *Given a graph* $G = (V(G), E(G))$ *and* $v \in V(G)$*, then* $i(G) = i_{-v}(G) + i_{+v}(G) = i(G - v) + i(G - N[v])$.

Lemma 1.2. ([6]) *If* H *is an edge-deletion of* G*, then* $i(G) < i(H)$.

Lemma 1.3. ([6]) *If* G *is the union of* $G_1, G_2, \ldots, G_k$*, then* $i(G) = \Pi_{j=1}^{k} i(G_j)$.

Lemma 1.4. ([6, 7]) *For an integer* $n \ge 2$*,* $i(P_n) = i(P_{n-1}) + i(P_{n-2})$*, where* $i(P_0) = 1$ *and* $i(P_1) = 2$.

Lemma 1.5. ([6]) *For an integer* $n \ge 5$*,* $i(C_n) = i(C_{n-1}) + i(C_{n-2})$*, where* $i(C_3) = 4$ *and* $i(C_4) = 7$.

Theorem 1.6. ([6, 7]) *If* T *is a tree of order* $n \ge 1$*, then* $i(T) \le 2^{n-1} + 1$. *Furthermore, the equality holds if and only if* $T = K_{1,n-1}$.

2. n-Vertex Graphs

Let $g(n, x)$ be the x-th largest number of independent sets among all n-vertex graphs and $G(n, x)$ be the n-vertex graphs achieving the number $g(n, x)$. In this section, we determine the numbers $g(n, x)$ for $1 \leq x \leq n$. Moreover, we also characterize the n-vertex graphs achieving these values.

Lemma 2.1. *Let G be a n-vertex graph.*

(i) *If G has at least one cycle, then $i(G) \leq 2^{n-1}$.*
(ii) *If G has a component which is not a star, then $i(G) \leq 2^{n-1}$.*
(iii) *If G have at least two nontrivial components such that $G \neq 2P_2 \cup (n-4)P_1$, then $i(G) < 2^{n-1}$.*

Proof. (i) If G has a cycle C_k, where $k \geq 3$, then $C_k \cup (n-k)P_1$ is an edge-deletion of G. By Lemma 1.5 and an induction, $i(C_k) \leq 2^{k-1}$. Then, by Lemmas 1.2 and 1.3, $i(G) \leq i(C_k \cup (n-k)P_1) \leq 2^{k-1}2^{n-k} = 2^{n-1}$. (ii) If G has a component H which is not a star, then $C_3 \cup (n-3)P_1$ or $P_4 \cup (n-4)P_1$ is an edge-deletion of G. By Lemmas 1.2 and 1.3, $i(G) \leq \min\{i(C_3 \cup (n-3)P_1), i(P_4 \cup (n-4)P_1)\} = 2^{n-1}$, since $i(C_3) = 4$ and $i(P_4) = 8$. (iii) If G have at least three nontrivial components, then $3P_2 \cup (n-6)P_1$ is an edge-deletion of G. By Lemma 1.2, $i(G) \leq i(3P_2 \cup (n-6)P_1) = 27 \cdot 2^{n-6} < 2^{n-1}$. Assume that G have exactly two nontrivial components. Note that $G \neq 2P_2 \cup (n-4)P_1$, then $P_3 \cup P_2 \cup (n-5)P_1$ is an edge-deletion of G. By Lemma 1.2 , $i(G) \leq i(P_3 \cup P_2 \cup (n-5)P_1) = 15 \cdot 2^{n-5} < 2^{n-1}$. ■

Note that $i(2P_2 \cup (n-4)P_1) = 9 \cdot 2^{n-4} > 2^{n-1}$ and $i(K_{1,x-1} \cup (n-x)P_1) = 2^{n-1} + 2^{n-x} > 2^{n-1}$, where $1 \leq x \leq n$. If $i(G) \geq 2^{n-1} + 1$, where $|G| = n$, by Lemma 2.1, then $G = 2P_2 \cup (n-4)P_1$ or $K_{1,x-1} \cup (n-x)P_1$.

Theorem 2.2. *For $1 \leq x \leq n$, $g(n, x) = (2^{x-1} + 1)2^{n-x} = 2^{n-1} + 2^{n-x}$ and*

$$G(n,x) = \begin{cases} K_{1,3} \cup (n-4)P_1 \textit{ or } 2P_2 \cup (n-4)P_1, & \textit{if } x = 4\,; \\ K_{1,x-1} \cup (n-x)P_1, & \textit{if } x \neq 4. \end{cases}$$

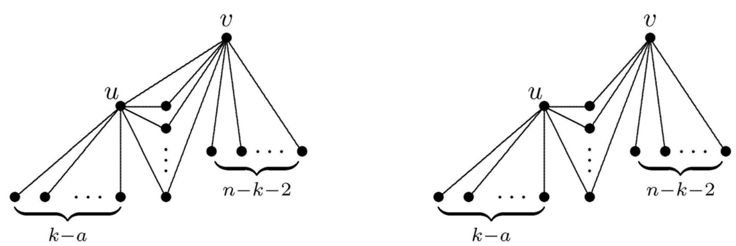
3. Connected n-Vertex Graphs

Let $h(n, x)$ be the x-th largest number of independent sets among all connected n-vertex graphs and $H(n, x)$ be the connected n-vertex graphs achieving the number $h(n, x)$. In this section, we determine the numbers $h(n, x)$ for $1 \leq x \leq \lfloor \frac{n}{2} \rfloor^2 - 3 \cdot \lfloor \frac{n}{2} \rfloor + 3$. Moreover, we also characterize the connected n-vertex graphs achieving these values. For $1 \leq k \leq \lfloor \frac{n}{2} \rfloor - 2$, let I_n^k be the interval $[2^{n-2} + 2^{n-k-2} + 1, 2^{n-2} + 2^{n-k-1}]$ and let ${}_n^k$ be the collection of all connected n-vertex graphs H having $i(H) \in I_n^k$.

Theorem 3.1. *For $n \geq 1$, $h(n, 1) = 2^{n-1} + 1$ and $H(n, 1) = K_{1,n-1}$.*

Proof. Suppose G is a connected n-vertex graph such that $i(G)$ as large as possible, by Lemma 1.2, $H(n,1)$ contains just a tree. By Theorem 1.6, $H(n,1) = K_{1,n-1}$ and $h(n,1) = 2^{n-1}+1$. ■

For $2 \le x \le \lfloor \frac{n}{2} \rfloor^2 - 3 \cdot \lfloor \frac{n}{2} \rfloor + 3$, we characterize the graphs $H(n,x)$ in Theorem 3.2. For this purpose, define graphs $H^1(n,k,a)$ and $H^2(n,k,a)$, see Figure 1. For $0 \le a \le k \le n-2$, the graphs $H^1(n,k,a)$ is the n-vertex graph containing an edge uv such that u and v have a common neighbors of degree 2, u has $k-a$ private neighbors of degree 1 and v has $n-k-2$ private neighbors of degree 1. The graph $H^2(n,k,a) = H^1(n,k,a) - uv$.



$H^1(n,k,a), 0 \le a \le k \le n-2.$ $H^2(n,k,a), 1 \le a \le k.$

Fig. 1. The graphs $H^1(n,k,a)$ and $H^2(n,k,a)$.

Theorem 3.2. *Let n and x be two nonnegative integers such that $2 \le x \le \lfloor \frac{n}{2} \rfloor^2 - 3 \cdot \lfloor \frac{n}{2} \rfloor + 3$. Suppose that $k = \lceil \frac{-1+\sqrt{4x-3}}{2} \rceil$ and $t = x - (k^2 - k + 1)$, then*

$$h(n,x) = \begin{cases} 2^{n-2} + 2^{n-k-2} + 2^{(k-\frac{t-1}{2})}, & \text{if } 1 \le t \le 2k-1 \text{ is odd;} \\ 2^{n-2} + 2^{n-k-2} + 2^{(k-\frac{t}{2})} + 1, & \text{if } 2 \le t \le 2k-2 \text{ is even;} \\ 2^{n-2} + 2^{n-k-2} + 1, & \text{if } t = 2k; \end{cases}$$

and

$$H(n,x) = \begin{cases} H^1(n,k,\frac{t-1}{2}), & \text{if } 1 \le t \le 2k-3 \text{ is odd;} \\ H^2(n,k,\frac{t}{2}), & \text{if } 2 \le t \le 2k-2 \text{ is even;} \\ H^1(n,k,k-1) \text{ or } H^2(n,k,k), & \text{if } t = 2k-1\,; \\ H^1(n,k,k), & \text{if } t = 2k. \end{cases}$$

The graphs in Figure 2 are the exceptional cases of $H(n,10)$, $H(n,12)$ and $H(n,13)$.

We prove the Theorem 3.2 by establishing the following lemmas.

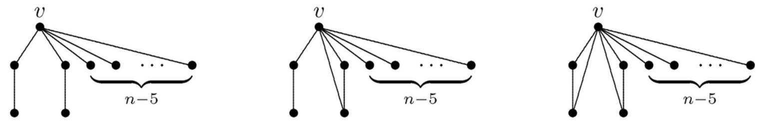


Fig. 2. The exceptional cases of $H(n,10)$, $H(n,12)$ and $H(n,13)$.

Lemma 3.3. *For $1 \leq k \leq \lfloor \frac{n}{2} \rfloor - 2$, if $H \in \mathcal{H}_n^k$ and v is a vertex of maximum degree in H such that $H - v \neq 2P_2 \cup (n-5)P_1$, then we have the following results.*
(i) $H - v = G(n-1, k+1)$.
(ii) $H - N[v] = sP_1$ $(0 \leq s \leq k)$ *or* $K_{1,t}$ *(*$1 \leq t \leq k-1$*).*
(iii) $i(H - N[v]) = 2^k, 2^{k-1}+1, 2^{k-1}, 2^{k-2}+1, \ldots, 2^1+1, 2^1 = 2^0+1, 1$.

Proof. Since $i(H) \leq 2^{n-2} + 2^{n-k-1}$ and $i(H - N[v]) \geq 1$, by Lemma 1.1, $i(H-v) = i(H) - i(H - N[v]) \leq 2^{n-2} + 2^{n-k-1} - 1$. By Theorem 2.2, $H - v = G(n-1, x)$, where $x \geq k+1$. Since $H - v \neq 2P_2 \cup (n-5)P_1$, $H - v = G(n-1, x) = K_{1,x-1} \cup (n-1-x)P_1$ for some $x \geq k+1$.

Claim. $x = k+1$. Assume that $x \geq k+2$, then $n - x \leq n-k-2$. Let $|N_H(v) \cap L(K_{1,x-1})| = a$, where $L(K_{1,x-1})$ is the set of leaves in $K_{1,x-1}$. So $i(H - N_H[v]) \leq 2^{x-1-a}+1$. Since v is a vertex of maximum degree in H, this implies that $x-1 \leq n-1-x+a$. Thus $x-1-a \leq n-1-x$. Thus $2^{n-2}+2^{n-k-2}+1 \leq i(H) = i(H-v) + i(H-N_H[v]) \leq (2^{x-1}+1)\cdot 2^{n-1-x} + 2^{x-1-a}+1 = 2^{n-2} + 2^{n-1-x}+2^{x-1-a}+1 \leq 2^{n-2}+2\cdot 2^{n-1-x}+1 = 2^{n-2}+2^{n-x}+1 \leq 2^{n-2}+2^{n-k-2}+1$, the equalities hold. Thus we got three equalities, $x = k+2$, $x-1-a = n-1-x$ and $i(H - N_H[v]) = 2^{x-1-a}+1$. Since $i(H-N_H[v]) = 2^{x-1-a}+1$, this means that u, the center of $K_{1,x-1}$, is not adjacent to v in H. By the connection property of H, so $a \geq 1$. Thus $n-1-(k+2) = n-1-x = x-1-a \leq (k+2)-1-1$, then $n-3 \leq 2k \leq 2\cdot(\lfloor \frac{n}{2} \rfloor - 2) \leq n-4$. This is a contradiction, hence $x = k+1$.

Then $H - v = G(n-1, k+1) = K_{1,k} \cup (n-k-2)P_1$ and $H - N[v] = sP_1$ $(0 \leq s \leq k)$ or $K_{1,t}$ $(1 \leq t \leq k-1)$. So $i(H - N[v]) = 2^k, 2^{k-1}+1, 2^{k-1}, 2^{k-2}+1, \ldots, 2^1+1, 2^1 = 2^0+1, 1$. ■

Suppose $H - v = 2P_2 \cup (n-5)P_1$, then $k = 3$ and $i(H - N_H[v]) = 1, 2$ or 4. Hence $H \in \mathcal{H}_n^3$, so $H \in H(n,10), H(n,12)$ or $H(n,13)$. The graphs in Figure 2 have the tenth, eleventh and thirteenth largest numbers of independent sets among all connected n-vertex graphs.

Lemma 3.4. *For $k \geq 1$, let $c(n,k) = |\{i(H); H \in \mathcal{H}_n^k, H - v \neq 2P_2 \cup (n-5)P_1\}|$. Then $|\mathcal{H}_n^k| = 2k+1$ and $c(n,k) = 2k$.*

Proof. By Lemma 3.3, we obtain that $|\mathcal{H}_n^k| = 2k+1$. Note that $i(H - N[v]) = i(P_1) = i(K_{1,0}) = 2$. Then $i(H - N[v]) = 2^k, 2^{k-1}+1, 2^{k-1}, 2^{k-2}+1, \ldots, 2^1+1, 2^1 = 2^0+1, 1$. Hence $c(n,k) = 2k$. ■

Lemma 3.5. *Let n and x be two nonnegative integers such that $x \leq \lfloor \frac{n}{2} \rfloor^2 - 3 \cdot \lfloor \frac{n}{2} \rfloor + 3$. Suppose that $H(n, x) \in \mathcal{H}_n^k$, then $k = \lceil \frac{-1+\sqrt{4x-3}}{2} \rceil$.*

Proof. By Lemma 3.4, $| \cup_{j=1}^{k-1} \mathcal{H}_n^j | = \Sigma_{j=1}^{k-1} c(n, j) = k^2 - k$ and $| \cup_{j=1}^{k} \mathcal{H}_n^j | = \Sigma_{j=1}^{k} c(n, j) = k^2 + k$. Note that $K_{1,n-1}$ is the connected n-vertex graph having the largest number of independent sets. If $H(n, x) \in \mathcal{H}_n^k$, then $k^2 - k + 1 < x \leq k^2 + k + 1$. Hence $k = \lceil \frac{-1+\sqrt{4x-3}}{2} \rceil$. ■

Theorem 3.2 then follows from Lemmas 3.3 to 3.5.

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