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MINIMUM GENERALIZATION DEGREE DISTANCE OF n-VERTEX UNICYCLIC AND BICYCLIC GRAPHS

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ABSTRACT. In [10] we introduced a generalization of degree distance of graphs as a new topological index. In this paper, we characterize the n-vertex unicyclic and bicyclic graphs which have the minimum generalization degree distance.

1 Introduction

Topological indices and graph invariants based on the distances between the vertices of a graph are widely used in theoretical chemistry to establish relations between the structure and the properties of molecules. They provide correlations with physical, chemical and thermodynamic parameters of chemical compounds [5, 19]. The Wiener index is a well-known topological index which equal to the sum of distances between all pairs of vertices of a molecular graph [22]. It is used to describe molecular branching and cyclicity and establish correlations with various parameters of chemical compounds. In this paper, we only consider simple and connected graphs. Let G be a connected graph with the vertex and edge sets $V(G)$ and $E(G)$, respectively and the number of vertices and edges of G are denoted respectively by n and m. As usual, the distance between the vertices u and v of G is denoted by $d_G(u, v)$ $(d(u, v)$

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for short). It is defined as the length of a minimum path connecting them. We let $d_G(v)$ be the degree of a vertex v in G. The eccentricity denoted by $\varepsilon(v)$ that is the maximum distance from vertex v to any other vertex. The diameter of a graph G is denoted by $diam(G)$ and is the maximum eccentricity over all vertices in a graph G. A connected graph G with n vertices and m edges is called unicyclic if $m = n$; G is called bicyclic if $m = n + 1$. The join $G = G_1 + G_2$ of two graphs G_1 and G_2 with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2 is the graph union $G_1 \cup G_2$ together with all the edges joining V_1 and V_2.

Additively weighted Harary index defined as follows in [1].

$$H_A(G) = \sum_{\{u,v\}\subseteq V(G)} d^{-1}(u,v)(d_G(u) + d_G(v)).$$

There are two papers [6, 7], which introduced a new graph invariant with the name degree distance. It is defined as follows:

$$D'\left(G\right) = \sum_{\{u,v\}\subseteq V(G)} d\left(u,v\right)\left(d_G\left(u\right) + d_G\left(v\right)\right).$$

The first Zagreb index was originally defined as $M_1(G) = \sum_{u\in V(G)} d_G(u)^2$ [8]. This index can be also expressed as a sum over edges of G, i.e., $M_1(G) = \sum_{uv\in E(G)}[d_G(u)+ d_G(v)]$. We refer the reader to [17] for the proof of this fact and for more information on Zagreb index. Generalization of degree distance denoted by $H_\lambda(G)$ and defined as follows in [10].

For every vertex x, $H_\lambda(x)$ is defined by $H_\lambda(x) = D^\lambda(x)d_G(x)$, where $D^\lambda(x) = \sum_{y\in V(G)} d^\lambda(x,y)$, and to avoid confusion,we show $H_\lambda(x)$ in graph G, with $H_\lambda(x,G)$. So we have:

$$H_\lambda(G) = \sum_{x\in V(G)} H_\lambda(x) = \sum_{x\in V(G)} D^\lambda(x)d_G(x) = \sum_{\{u,v\}\subseteq V(G)} d^\lambda(u,v)(d_G(u) + d_G(v)),$$

where λ is a real number. If $\lambda = 0$, then $H_\lambda(G) = 4m$. Since for $\lambda = 1$, this new topological index ($H_\lambda(G)$) is equal to degree distance (or Schultz index), there are many papers for study this topological index. For example see [4, 12, 20, 21], and also if $\lambda = -1$, then $H_\lambda(G) = H_A(G)$. Therefore the study of this new topological index is important and we try obtain some new results related to this topological index.

Throughout this paper, C_n, K_n and $K_{1,n-1}$ denote the cycle, complete and star graphs on n vertices respectively. Our other notations are standard and taken mainly from [5, 9, 19].

Extremal graph theory is a branch of the mathematical field of graph theory. Extremal graph theory studies extremal (maximal or minimal) graphs which satisfy a certain property. Extremality can be taken with respect to different graph invariants, such as order, size or girth. The problem of determining extremal values and corresponding extremal graphs of some graph invariants is the topic of several papers for example see [2–4, 12, 14, 15, 20, 21]. In [23], the authors compared the energy of two unicyclic molecular graphs.

In this paper, we characterize all of n-vertex unicyclic and bicyclic graphs which have the minimum generalization degree distance.

2 Main Results

It is well known, that natural numbers $d_1 \geq d_2 \geq \ldots \geq d_n \geq 1$ are the degrees of the vertices of a tree if and only if $\sum_{i=1}^{n} d_i = 2n - 2$, [16, 18]. The next two lemmas characterize connected unicyclic and bicyclic graphs by their degree sequence.

Lemma 2.1. [20] Let $n \geq 3$ and G be a n-vertex unicyclic graph. The integers $d_1 \geq d_2 \geq \ldots \geq d_n \geq 1$ are the degrees of the vertices of a graph G if and only if
(i) $\sum_{i=1}^{n} d_i = 2n$,
(ii) at least three of them are greater than or equal to 2.

Lemma 2.2. [20] Let $n \geq 4$ and G be a n-vertex bicyclic graph. The integers $d_1 \geq d_2 \geq \ldots \geq d_n \geq 1$ are the degrees of the vertices of a graph G if and only if
(i) $\sum_{i=1}^{n} d_i = 2n + 2$,
(ii) at least four of them are greater than or equal to 2,
(iii) $d_1 \leq n - 1$.

Let x_i be the number of vertices of degree i of G, for $1 \leq i \leq n-1$. If $d_G(v) = k$, then

$$D^{\lambda}(v) = \sum_{u \in V(G)} d^{\lambda}(u,v) \quad = \sum_{u \in V(G), d(u,v)=1} d^{\lambda}(u,v) + \sum_{u \in V(G), d(u,v) \geq 2} d^{\lambda}(u,v)$$

$$\begin{aligned} &\geq k + 2^{\lambda}(n-k-1) \\ &= 2^{\lambda}n - k(2^{\lambda}-1) - 2^{\lambda}, \end{aligned}$$

so

$$\begin{aligned} H_{\lambda}(G) &= \sum_{v \in V(G)} d_G(v) D^{\lambda}(v) \\ &\geq \sum_{k=1}^{n-1} k x_k (2^{\lambda}n - k(2^{\lambda}-1) - 2^{\lambda}). \end{aligned}$$

We define

$$F_{\lambda}(x_1, x_2, \ldots, x_{n-1}) = \sum_{k=1}^{n-1} k x_k (2^{\lambda}n - k(2^{\lambda}-1) - 2^{\lambda}).$$

We obtain the minimum of $F_{\lambda}(x_1, x_2, \ldots, x_{n-1})$ over all integers numbers $x_1, x_2, \ldots, x_{n-1} \geq 0$ which satisfy one of the conditions of Lemmas 2.1 and 2.2. Rewriting Lemmas 2.1 and 2.2 in terms of the above notations, as follows:

Corollary 2.3. [20] Let $n \geq 3$ and G be a n-vertex unicyclic graph. The integers $x_1, x_2, \ldots, x_{n-1} \geq 0$ are the multiplicities of the degrees of a graph G if and only if
(i) $\sum_{i=1}^{n-1} x_i = n$,
(ii) $\sum_{i=1}^{n-1} i x_i = 2n$,
(iii) $x_1 \leq n-3$.

We denote the set of all vectors $(x_1, \ldots, x_{n-1})$ which satisfy the above conditions by B_1.

Corollary 2.4. [20] Let $n \geq 4$ and G be a n-vertex bicyclic graph. The integers $x_1, x_2, \ldots, x_{n-1} \geq 0$ are the multiplicities of the degrees of a graph G if and only if
(i) $\sum_{i=1}^{n-1} x_i = n$,
(ii) $\sum_{i=1}^{n-1} i x_i = 2n+2$,
(iii) $x_1 \leq n-4$.

We denote the set of all vectors $(x_1, \ldots, x_{n-1})$ which satisfy the above conditions by B_2.

Let G be a connected graph with multiplicities of the degrees $(x_1, \ldots, x_{n-1})$ and let $m \geq 2$, $p > 0$, $m + p \leq n-2$, $x_m \geq 1$ and $x_{m+p} \geq 1$. Now we consider the transformation of t_1 which defined as follows [20]:

$$\begin{aligned} t_1(x_1,\dots,x_{n-1}) &= (x'_1,\dots,x'_{n-1}) \\ &= (x_1,\dots,x_{m-1}+1,x_m-1,\dots,x_{m+p}-1,x_{m+p+1}+1,\dots,x_{n-1}). \end{aligned}$$

We have $x'_i = x_i$ for $i \notin \{m-1,m,m+p,m+p+1\}$ and $x'_{m-1} = x_{m-1}+1$, $x'_m = x_m - 1$, $x'_{m+p} = x_{m+p}-1$, $x'_{m+p+1} = x_{m+p+1}+1$.

Let $2 \le m \le n-2$, $x_m \ge 2$. Now consider the transformation t_2 defined as follows [20]:

$$\begin{aligned} t_2(x_1,\dots,x_{n-1}) &= (x'_1,\dots,x'_{n-1}) \\ &= (x_1,\dots,x_{m-1}+1,x_m-2,x_{m+1}+1\dots,x_{n-1}). \end{aligned}$$

That is $x'_i = x_i$ for $i \notin \{m-1,m,m+1\}$ and $x'_{m-1} = x_{m-1}+1$, $x'_m = x_m-2$, $x'_{m+1} = x_{m+1}+1$.

Lemma 2.5. Suppose that λ is a positive integer number and consider the set of vectors $(x_1,\dots,x_{n-1})$.

1) If $(x_1,\dots,x_{n-1}) \in B_1$, then $t_1(x_1,\dots,x_{n-1}) \in B_1$ unless $m=2$ and $x_1 = n-3$,

2) If $(x_1,\dots,x_{n-1}) \in B_2$, then $t_1(x_1,\dots,x_{n-1}) \in B_2$ unless $m=2$ and $x_1 = n-4$,

3) $F_\lambda(t_1(x_1,x_2,\dots,x_{n-1})) < F_\lambda(x_1,x_2,\dots,x_{n-1})$.

Proof. (1) We can easily see that $\sum_{i=1}^{n-1} x_i = \sum_{i=1}^{n-1} x'_i$, $\sum_{i=1}^{n-1} ix_i = \sum_{i=1}^{n-1} ix'_i$. If $m=2$, $x_1 = n-3$, then $x'_1 > n-3$, and in this case $t_1(x_1,\dots,x_{n-1}) \notin B_1$. Now if $x'_1 > n-3$, according to $x_1 \le n-3$, we have $m=2$ and $x_1 = n-3$. Therefore, we conclude that if $(x_1,\dots,x_{n-1}) \in B_1$, then $x'_1 > n-3$ if and only if $m=2$ and $x_1 = n-3$.

(2) With a similar argument, if $(x_1,\dots,x_{n-1}) \in B_2$, then $x'_1 > n-4$ if and only if $m=2$ and $x_1 = n-4$.

(3) With a simple calculation we have:

$$\begin{aligned} F_\lambda(x_1,x_2,\dots,x_{n-1}) - F_\lambda(t_1(x_1,x_2,\dots,x_{n-1})) &= (2^\lambda - 1)(2p+2) \\ &> 0. \end{aligned}$$

The proof is now completed. $\square$

Lemma 2.6. Suppose that λ is a positive integer number and consider the set of vectors $(x_1, \ldots, x_{n-1})$.
1) If $(x_1, \ldots, x_{n-1}) \in B_1$, then $t_2(x_1, \ldots, x_{n-1}) \in B_1$ unless $m = 2$ and $x_1 = n - 3$,
2) If $(x_1, \ldots, x_{n-1}) \in B_2$, then $t_2(x_1, \ldots, x_{n-1}) \in B_2$ unless $m = 2$ and $x_1 = n - 4$,
3) $F_\lambda(t_2(x_1, x_2, \ldots, x_{n-1})) < F_\lambda(x_1, x_2, \ldots, x_{n-1})$.

Proof. The proof is similar to the proof of the previous lemma, by taking $p = 0$. $\square$

Theorem 2.7. Let $n \geq 3$ and λ be a positive integer number. If G is belong to the classes of connected unicyclic graphs with n vertex, then we have:

$$\min H_\lambda(G) = 2^\lambda(n^2 - n - 6) + (n^2 - n + 6),$$

and the unique extremal graph is $K_{1,n-1} + e$ where $e \in E(\bar{K}_{1,n-1})$.

Proof. To find minimum $H_\lambda(G)$, over the classes of connected unicyclic graphs with n vertex, it is enough to find $\min_{(x_1,x_2,\ldots,x_{n-1}) \in B_1} F_\lambda(x_1, x_2, \ldots, x_{n-1})$. At first, we consider the case n = 3. In this case only unicyclic graph with 3 vertices is C_3, that $H_\lambda(C_3) = 12 = \theta(3)$, where $\theta(n) = 2^\lambda(n^2-n-6)+(n^2-n+6)$, moreover $C_3 = K_{1,2}+e$ where $e \in E(\bar{K}_{1,2})$ and the theorem is proved in this case. $\square$

Now let $n \geq 4$. If $x_{n-1} \geq 2$, consider two different vertices $x, y \in V(G)$ such that $d_G(x) = d_G(y) = n - 1$. Since $n \geq 4$, we can choose two different vertices $z, t \in V(G) - \{x, y\}$. We have $xy, xz, xt, yz, yt \in E(G)$, hence graph G has at least two cycles x, y, z, x and x, y, t, x, which contradicts the hypothesis. Therefore $x_{n-1} \leq 1$.

Let us analyze the possible values for $x_3, \ldots, x_{n-2}$ in the case of minimum. If there exist $3 \leq i < j \leq n - 2$ such that $x_i \geq 1$ and $x_j \geq 1$, then by applying t_1 for the positions i and j, we obtain a new vector $(x'_1, \ldots, x'_{n-1}) \in B_1$ such that $F_\lambda(x'_1, x'_2, \ldots, x'_{n-1}) < F_\lambda(x_1, x_2, \ldots, x_{n-1})$. Similarly, if there exists $3 \leq i \leq n - 2$ such that $x_i \geq 2$, then by t_2 we obtain a new degree sequence in B_1 such that $F_\lambda(x'_1, x'_2, \ldots, x'_{n-1}) < F_\lambda(x_1, x_2, \ldots, x_{n-1})$. Two remaining cases are (a) $x_3 = x_4 = \cdots = x_{n-2} = 0$ and (b) there is only one index i, $3 \leq i \leq n - 2$ such that $x_i = 1$ and $x_k = 0$ for all $3 \leq k \leq n - 2, k \neq i$. In follow, we prove that, the minimum of $F_\lambda(x_1, x_2, \ldots, x_{n-1})$ does not occur in case (b). Let $x_2 = 0$, with considering the case (b), we have $x_1 + x_{n-1} = n - 1$. Since $x_{n-1} \leq 1$, if $x_{n-1} = 0$, then $x_1 = n - 1$ and if $x_{n-1} = 1$, then $x_1 = n - 2$, but both of them is inconsistent with condition (iii) from Corollary 2.3, so $x_2 \geq 1$. Let $x_1 > n - 4$. By applying conditions (i) and (iii) from Corollary 2.3, we have $x_1 = n-3$, $n-3+x_2+1+x_{n-1} = n$. Now by applying condition (ii) from Corollary 2.3, we obtain $n - 3 + 2x_2 + i + (n - 1)x_{n-1} = 2n$, or equivalent $n+4+(i-3)+(n-3)x_{n-1} = 2n$, by the fact that $i \geq 3$ leads to $(n-3)x_{n-1} \leq n-4$. If $x_{n-1} = 0$, then $x_2 = 2$ and we deduce $i = n-1$,that is a contradiction. If $x_{n-1} = 1$, then $x_2 = 1$ and we deduce $i = 2$, that is a contradiction. Finally, $x_1 \leq n-4$ and now it is possible to apply t_1 for positions 2 and i, obtaining a new vector $(x'_1, \ldots, x'_{n-1}) \in B_1$ for which $F_\lambda(x'_1, x'_2, \ldots, x'_{n-1}) < F_\lambda(x_1, x_2, \ldots, x_{n-1})$. Therefore case (b) is not hold and therefore case (a) holds, thus implying $x_3 = \cdots = x_{n-2} = 0$. The degree sequence at this point is $(x_1, x_2, 0, \ldots, 0, x_{n-1})$ with $x_{n-1} \in \{0, 1\}$. Let us consider the case $x_{n-1} = 0$. We have $x_1 + x_2 = n$ and $x_1 + 2x_2 = 2n$, implying that $x_2 = n$ and $x_1 = 0$. In this case, $(0, n, 0, ..., 0)$ cannot be a point of minimum in B_1 since transformation t_2 can be applied to this vector. The remaining case is $x_{n-1} = 1$. Conditions (i) and (ii) of Corollary 2.3 imply that $x_2 = 2$ and $x_1 = n-3$. It follows that $F_\lambda(x_1, x_2, \ldots, x_{n-1})$ is minimum if and only if $x_1 = n - 3, x_2 = 2, x_3 = \cdots = x_{n-2} = 0, x_{n-1} = 1$ and the corresponding graph is $K_{1,n-1} + e$ where $e \in E(\bar{K}_{1,n-1})$. Hence,

$$
\begin{aligned}
\min H_\lambda(G) &\geq \min_{(x_1,x_2,\ldots,x_{n-1})\in B_1} F_\lambda(x_1, x_2, \ldots, x_{n-1}) \\
&= F_\lambda(n-3, 2, 0, \ldots, 0, 1) \\
&= 2^\lambda(n^2 - n - 6) + (n^2 - n + 6) \\
&= H_\lambda(K_{1,n-1} + e)
\end{aligned}
$$

and the proof is completed. □

In [20], the authors proved that the following Theorem.

Theorem 2.8. For every $n \geq 3$ we have

$$\min D'(G) = 3n^2 - 3n - 6,$$

that G is belong to the classes of connected unicyclic graphs with n vertex and the unique extremal graph is $K_{1,n-1} + e$.

If we choose $\lambda = 1$ in Theorem 2.7, then we can obtain the same result (Theorem 3.1 in [20]).

Theorem 2.9. Let $n \geq 4$ and λ be a positive integer. If G is belong to the classes of connected bicyclic graphs with n vertex, then we have:

$$\min H_\lambda(G) = 2^\lambda(n^2 + n - 16) + (n^2 - n + 14),$$

the extremal graph is unique and obtained from $K_{1,n-1}$ by adding two edges having a common extremity.

Proof. To find minimum $H_\lambda(G)$, over the classes of connected bicyclic graphs with n vertex, it is enough to find $\min_{(x_1,x_2,\ldots,x_{n-1})\in B_2} F_\lambda(x_1, x_2, \ldots, x_{n-1})$. At first, we consider the case n = 4. In this case only bicyclic graph with 4 vertices is $C_4 + e$, that $H_\lambda(C_4 + e) = 26 + 4.2^\lambda = \theta(4)$, where $\theta(n) = 2^\lambda(n^2 + n - 16) + (n^2 - n + 14)$, and the theorem is proved in this case.

Now let $n \geq 5$. Similar to the proof of the previous Theorem, we have, $x_{n-1} \leq 1$. Similarly, on positions $4, \ldots, n-2$, we cannot have two values greater than or equal to 1 or one value greater than or equal to 2. Let us show that all vectors $(x_1, \ldots, x_{n-1}) \in B_2$ realizing the minimum of F_λ have $x_4 = x_5 = \cdots = x_{n-2} = 0$.

Let there exist $4 \leq i \leq n-2$ such that $x_i = 1$ and $x_k = 0$ for $k \neq i$, $4 \leq k \leq n-2$. In this case, if $x_3 \geq 1$, then by applying t_1 for the positions i and 3, we obtain a new vector $(x'_1, \ldots, x'_{n-1}) \in B_2$ such that $F_\lambda(x'_1, x'_2, \ldots, x'_{n-1}) < F_\lambda(x_1, x_2, \ldots, x_{n-1})$. Let $x_3 = 0$, since $x_{n-1} \in \{0, 1\}$, we consider two cases, (a) $x_{n-1} = 1$ and (b) $x_{n-1} = 0$. In case (a), for $i \geq 4$, we have $x_{n-1} = x_i = 1$. We can consider different vertices $x, y, u, v, w \in V(G)$ such that $d_G(x) = n - 1 \geq 4, d_G(y) = i \geq 4$, $xy, xu, xv, xw, yu, yv, yw \in E(G)$. We have found three linearly independent cycles x, y, u, x; x, y, v, x; x, y, w, x, which contradicts the hypothesis about G. In case (b), if $x_{n-1} = 0$, then with conditions B_2, we have, $x_1 + x_2 = n - 1$, $x_1 + 2x_2 + i = 2n + 2$ and $x_1 \leq n - 4$. We deduce that $x_1 = i - 4 \leq n - 6$ and $x_2 = n + 3 - i \geq 1$. In this case we can apply t_1 for positions 2 and i and deduce a smaller value for F_λ. Therefore, $x_4 = x_5 = \cdots = x_{n-2} = 0$, $x_{n-1} \in \{0, 1\}$. If $x_{n-1} = 0$, then $x_1 + x_2 = n - x_3$, $x_1 + 2x_2 = 2n + 2 - 3x_3$, therefore $x_3 \geq 2$. By applying t_2 for the position 3, we obtain a smaller value for F_λ. If $x_{n-1} = 1$, then $x_1 + x_2 + x_3 = n - 1$,

$x_1+2x_2+3x_3 = n+3$. If $x_3 = 0$ we obtain $(n-5, 4, 0, \ldots, 0, 1) \in B_2$ and if $x_3 = 1$ we get $(n-4, 2, 1, 0, \ldots, 0, 1) \in B_2$. But $(n-4, 2, 1, 0, \ldots, 0, 1) = t_2(n-5, 4, 0, \ldots, 0, 1)$. It follows that $F_\lambda(x_1, x_2, \ldots, x_{n-1})$ is minimum in B_2 if and only if $x_1 = n-4$, $x_2 = 2$, $x_3 = 1$, $x_4 = \cdots = x_{n-2} = 0$ and $x_{n-1} = 1$. The corresponding graph is $K_{1,n-1} + 2e$, where the additional edges have a common extremity. This graph has also diameter 2. As in Theorem 2.7, we have:

$$\begin{aligned}
\min H_\lambda(G) &\geq \min_{(x_1,x_2,\ldots,x_{n-1})\in B_2} F_\lambda(x_1, x_2, \ldots, x_{n-1}) \\
&= F_\lambda(n-4, 2, 1, 0, \ldots, 0, 1) \\
&= 2^\lambda(n^2+n-16) + (n^2-n+14) \\
&= H_\lambda(K_{1,n-1}+2e)
\end{aligned}$$

and the proof is completed. □

In [20], the authors proved that the following Theorem.

Theorem 2.10. For every $n \geq 4$ we have

$$\min D'(G) = 3n^2 + n - 18,$$

that G is belong to the classes of connected bicyclic graphs with n vertex. The extremal graph is unique and obtained from $K_{1,n-1}$ by adding two edges having a common extremity.

If we choose $\lambda = 1$ in Theorem 2.9, then we can obtain the same result (Theorem 3.2 in [20]).

Let ${K_n}^p$ be the graph obtained by attaching p pendent edges to a vertex of K_{n-p}. We first bring the following results in [11, 13].

Lemma 2.11. [13] Let G be an n-vertex connected graph with p pendent vertices. Then $M_1(G) \leq n^3 - (3p-1)n^2 + (3p^2+6p+1)n - p^3 - 3p^2 - 2p - 1$, the equality is hold if and only if $G \cong {K_n}^p$.

Lemma 2.12. [10] Let G be a connected graph of order $n \geq 2$ and size $m \geq 1$ and λ be a negative integer. Then $H_\lambda(G) \leq (1-2^\lambda)M_1(G) + 2^{\lambda+1}mn - 2^{\lambda+1}m$ and equality is hold if and only if $d \leq 2$, where d is the diameter of G.

Lemma 2.13. [13] Let G be a connected graph with at least three vertices and λ be a negative integer. If G is not isomorphic to K_n, then $H_\lambda(G) < H_\lambda(G+e)$, where $e \in E(\bar{G})$.

Theorem 2.14. Let G be an n-vertex connected graph with p pendent vertices. Then

$$\begin{aligned} H_\lambda(G) &\leq n^3-(3p-1)n^2+(3p^2+6p+1)n-p^3-3p^2-2p-1 \\ &+ 2^\lambda(-3n^2-2p^2n-5np+2p^2+3pn^2+p^3+1-p)+2^{\lambda+1}(2np-n^2p), \end{aligned}$$

the equality is hold if and only if $G \cong K_n{}^p$.

Proof. Since G is an n-vertex connected graph with p pendent vertices, then the maximum number of edges in the graph G is equal to $p+\frac{(n-p)(n-p-1)}{2}$ and we know that the graph $K_n{}^p$ has $p+\frac{(n-p)(n-p-1)}{2}$ edges. By the above lemmas, we have:

$$\begin{aligned} H_\lambda(G) &\leq (1-2^\lambda)M_1(G)+2^{\lambda+1}mn-2^{\lambda+1}m \\ &\leq n^3-(3p-1)n^2+(3p^2+6p+1)n-p^3-3p^2-2p-1 \\ &+ 2^\lambda(-3n^2-2p^2n-5np+2p^2+3pn^2+p^3+1-p)+2^{\lambda+1}(2np-n^2p), \end{aligned}$$

The first equality holds if and only if the diameter of G is at most 2 and the second one holds if and only if $G \cong K_n{}^p$. Note that $K_n{}^p$ has diameter 2. So, the equality is hold if and only if $G \cong K_n{}^p$. This completes the proof. $\square$

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 $\beta = \max\{|S| : S$ is an independent set of $G\}$ is said to be the independence number of G. A clique of a graph is a maximal complete subgraph.

Theorem 2.15. Let G be an n-vertex connected graph with independence number β and λ be a negative integer. Then $H_\lambda(G) \leq (n-\beta)(n\beta-\beta^2+(n-1)^2+2^\lambda(\beta^2-\beta))$, and the equality is hold if and only if $G \cong \beta K_1 + K_{n-\beta}$.

Proof. Let G be a graph chosen among all n-vertex connected graphs with independence number β such that G has the largest $H_\lambda(G)$. Let S be a maximal independent set in G with $|S| = \beta$. Since adding edges into a graph will increase its $H_\lambda(G)$ by

Lemma 2.13, the subgraph induced by vertices in $G - S$ is a clique in G, moreover each vertex x in S is adjacent to every vertex y in $G - S$, then $G \cong \beta K_1 + K_{n-\beta}$. An elementary calculation gives $H_\lambda(G) \leq (n-\beta)(n\beta - \beta^2 + (n-1)^2 + 2^\lambda(\beta^2 - \beta))$, and the proof is completed. $\square$

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