The eccentric distance sum, the Harary index and the degree powers of graphs with given diameter *

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Abstract: Let G be a simple connected graph with the vertex set $V(G)$. The eccentric distance sum of G is defined as $\xi^d(G) = \sum_{v \in V(G)} \varepsilon(v) D_G(v)$, where $\varepsilon(v)$ is the eccentricity of the vertex v and $D_G(v)$ is the sum of all distances from the vertex v. The Harary index of G is defined as $H(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d(u,v)}$, where $d(u,v)$ is the distance between u and v in G. The degree powers of G is defined as $F_p(G) = \sum_{v \in V(G)} d(u)^p$ for the natural number $p \geq 1$. In this paper, we determine the extremal graphs with the minimal eccentric distance sum, the maximal Harary index and the maximal degree powers among all graphs with given diameter.

1 Introduction

Let G be a simple connected graph with the vertex set $V(G)$. For a vertex $v \in V(G)$, we use $N(v)$ to denote the set of vertices adjacent to v, $N[v] = N(v) \cup \{v\}$, $d_G(v)$ (or $d(v)$ for abbreviation) denotes the degree of v. For $S \subseteq V(G)$, $N(S)$ denotes the set of vertices adjacent to some vertex in S. For vertices $u, v \in V(G)$, the *distance* $d(u,v)$ is defined as the length of a shortest path between u and v in G, and $D_G(v) = \sum_{u \in V(G)} d(u,v)$ (or $D(v)$ for short). The *eccentricity* $\varepsilon(v)$ of a vertex v is the maximum distance from v to any other vertex. The *diameter* $d(G)$ of a graph is the maximum eccentricity of any vertex in G. Let S_n and P_n be a star and a path on n vertices, respectively.

Let $\mathcal{G}_{n,D}$ be the set of connected graphs of order n with given diameter D. Let $G \in \mathcal{G}_{n,D}$. Obviously, if $D = 1$, then G is the complete graph K_n. If $D = n-1$,

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then G is the path P_n. Therefore, in the rest of this paper we always assume $2 \leq D \leq n-2$.

The eccentric distance sum of G (EDS) is defined as [13]

$$\xi^d(G) = \sum_{v \in V(G)} \varepsilon(v) D_G(v).$$

As a topological index, $\xi^d(G)$ was successfully used for mathematical models of biological activities of diverse nature [27, 28]. In [30], the authors investigated the eccentric distance sum of unicyclic graphs with given girth and characterized the extremal graphs with the minimal and the second minimal eccentric distance sum. Furthermore, the authors characterized the extremal trees with minimal eccentric distance sum of trees with given diameter. The present authors in [14, 18] determined the extremal trees with maximal eccentric distance sum and established various lower and upper bounds for the eccentric distance sum in terms of many graph invariants.

The Harary index is defined as the half-sum of the elements in the reciprocal distance matrix (also called the Harary matrix [16]), more precisely

$$H(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d(u,v)}.$$

After its appearance, research regarding to the Harary index of a graph attracts much attention. Gutman [10] supported the use of Harary index as a measure of branching in alkanes. In [34], Zhou et al. presented some lower and upper bounds for the Harary index of connected graphs, triangle-free and quadrangle-free graphs and established the Nordhaus-Gaddum type inequalities. Yu and Feng [31] investigated the Harary index for a class of bicyclic graphs and characterized the extremal graphs. Ilić, Yu and Feng [15] investigated the Harary index of trees in terms of the number of pendent vertices and other graph invariants. For the history of Harary index, one may refer to [23]. In [8], the authors obtained a few lower and upper bounds for the Harary index of graphs in terms of diameter. But they did not get the extremal graph with the maximal Harary index among all graphs with given diameter.

The inverse degree $r(G)$ of G is defined as $r(G) = \sum_{u \in V(G)} \frac{1}{d(u)}$. The inverse degree first attracted attention through numerous conjectures generated by the Graffiti [9]. Since then its relationship with other graph invariants, such as diameter [5, 19, 24], edge-connectivity [6], matching number [33] is studied. Li and Zhao [20], Zhang and Zhang [32], and Chen and Deng [4] obtained sharp upper and lower bounds for the inverse degree of trees, unicyclic graphs and bicyclic graphs, respectively (see also [11, 29] for further results). Caro and Yuster [2] defined the *degree powers* $F_p(G)$ of a graph G as

$$F_p(G) = \sum_{v\in V(G)} d(u)^p$$

for the natural number $p \geq 1$.

In light of the information available for the sums of degree powers, several classes are considered such as trees, unicyclic graphs [11], bicyclic graphs [4], (m, n) graphs [12, 25], graphs with extremal properties [1, 2, 3, 26], it is natural to consider other classes of graphs. In [17], Li and Yan considered the degree powers of graphs with k cut edges, this impulses us to consider the similar problem for graphs with a given diameter. To the best of our knowledge, this is not considered so far.

This paper is organized as follows. In Section 2, we present some preliminary results that will be used later. In Sections 3, 4, 5, we study the eccentric distance sum, the Harary index and the degree powers of graphs with given diameter, respectively.

2 Preliminaries

The following lemma is easy to verify.

Lemma 2.1. *Let G be a non-complete connected graph and e is an edge in $\overline{G}$ (the complement of G). Then $\xi^d(G) > \xi^d(G+e)$, $H(G) < H(G+e)$, $F_p(G) < F_p(G+e)$*

Lemma 2.2. *[17] Let u and v be two vertices of G. Suppose $v_1, v_2, \ldots, v_s \in N(v) \setminus N[u]$ $(1 \leq s \leq d_G(v))$ and $u_1, u_2, \ldots, u_t \in N(u) \setminus N[v]$ $(1 \leq t \leq d_G(u))$. Let $G' = G - \{vv_1, vv_2, \ldots, vv_s\} + \{uv_1, uv_2, \ldots, uv_s\}$, $G'' = G - \{uu_1, uu_2, \ldots, uu_t\} + \{vu_1, vu_2, \ldots, vu_t\}$. Then we have, if $d_G(u) \geq d_G(v)$ then $F_p(G') > F_p(G)$; if $d_G(u) < d_G(v)$ then $F_p(G'') > F_p(G)$.*

Lemma 2.3. *Let $G \in \mathcal{G}_{n,D}$ be a connected graph of order n with diameter D $(2 \leq D \leq n-2)$. If G has the minimal EDS (resp. maximal $F_p(G)$), then G is the graph obtained from the path P_{D+1} by replacing the vertices by cliques, such that the vertices in distinct cliques are adjacent if and only if the corresponding original vertices in the path are adjacent. Moreover, the cliques corresponding to the endvertices have size 1.*

Proof. The proof of the result is similar to Lemma 1 in [7]. We only present the proof regarding EDS. Consider a graph with minimal EDS among the graphs of order n with diameter D. Let v_0 and v_D be the vertices of G at distance D. Let V_i be the set of vertices at distance i from v_0, $i = 0, 1, \dots, D$. If the graph is not of the claimed form, then one of the sets V_i contains two vertices that are not adjacent, or there is a vertex in V_i and a vertex in V_{i+1} that are not adjacent, or the set V_D contains more than one vertex. The first two cases are impossible, since adding the missing edge decreases the EDS from Lemma 2.1 and leaves the diameter unchanged. In the last case we get a contradiction, since adding edges between all but one vertex of V_D and all vertices of V_{D-2} decreases the EDS, and leaves the diameter unchanged. □

Let $G \in \mathcal{G}_{n,D}$ be the graph with minimal EDS (resp. maximal $F_p(G)$). According to Lemma 2.3 it consists of "pathwise adjacent cliques". Let us call these cliques *distance layers* and denote by V_i, $i = 0, 1, \dots, D$, ordered such that all vertices of V_i are adjacent to all vertices of V_{i+1} for $i = 0, 1, \dots, D-1$. Let n_i be the size of V_i. From Lemma 2.3, we have $n_0 = n_D = 1$.

Suppose the vertex in N_0 and N_D is u and v, respectively.

From Lemma 2.1, if $D = 2$, then the graph with extremal $F_p(G)$ is the graph obtained from the complete graph by deleting one edge. So in the rest of the section, we assume that $D \geq 3$.

For $\overline{K_2} = \{u, v\}$, $l_1 \geq l_2$ and $l_1 + l_2 = D - 2$, the graph G_{l_1,l_2} (as shown in Fig. 1) is obtained from $K_{n-D} \vee \overline{K_2}$ (the join of K_{n-D} and $\overline{K_2}$) by identifying one endvertex of each path of length l_1 and l_2 with u and v, respectively. It is easy to see that G_{l_1,l_2} has diameter D. If $l_1 - l_2 \leq 1$, we denote the graph by G^*_D.

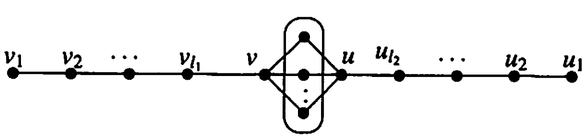

Figure 1. The graph G_{l_1,l_2}.

For odd D, denote by $\mathcal{G}^{\blacklozenge}_D$ the set of graphs obtained from $K_k \vee K_{n-D+1-k}$ by connecting an endvertex of a path $P_1 = P_{(D-1)/2}$ with all vertices from K_k and connecting an endvertex of a path $P_2 = P_{(D-1)/2}$ with all vertices from $K_{n-D+1-k}$, where $1 \leq k \leq n - D$.

3 Minimal eccentric distance sum of graphs

At first, we calculate the exact values of eccentric distance sum of G_D^* for even D and $G \in \mathcal{G}_D^\blacklozenge$

When D is even, assume that $P_{D+1} = v_0 v_1 \cdots v_D$ be a diametrical path in G_D^*. We divide the vertex set $V(G_D^*)$ into three parts: $U_1 = \{v_0, v_1, \ldots, v_{\frac{D}{2}-1}\}$, $U_2 = \{v_{\frac{D}{2}+1}, \ldots, v_D\}$ and the central layer $U_3 = V_{\frac{D}{2}}$. It follows that

- For $v_i \in U_1$: $\varepsilon(v_i) = D - i$ and $D(v_i) = \frac{i(i+1)}{2} + \frac{(D-i)(D-i+1)}{2} + (\frac{D}{2} - i)(n - D - 1)$;
- For $v_i \in U_2$: $\varepsilon(v_i) = i$ and $D(v_i) = \frac{i(i+1)}{2} + \frac{(D-i)(D-i+1)}{2} + (i - \frac{D}{2})(n - D - 1)$;
- For $v \in U_3$: $\varepsilon(v) = \frac{D}{2}$ and $D(v) = \frac{D(D+2)}{4} + n - D - 1$.

Therefore, it follows that

$\xi^d(G_D^*) = \sum_{i=0}^{\frac{D}{2}-1}(D-i)\left[\frac{i(i+1)}{2} + \frac{(D-i)(D-i+1)}{2} + (\frac{D}{2} - i)(n - D)\right]$
$+ \sum_{j=\frac{D}{2}+1}^{D} j\left[\frac{j(j+1)}{2} + \frac{(D-j)(D-j+1)}{2} + (j - \frac{D}{2})(n - D)\right] + \frac{D(n-D)}{2}\left[\frac{D(D+2)}{4} + n - D - 1\right]$
$= -\frac{1}{96}D\left[7D^3 - (32n + 28)D^2 + (24n - 28)D - 48n^2 + 32n + 16\right].$

Similarly, if D is odd, for any $G \in \mathcal{G}_D^\blacklozenge$, one has

$\xi^d(G) = -\frac{D+1}{96}\left[7D^3 - (32n + 23)D^2 + (44n + 1)D - 48n^2 + 36n + 15\right].$

ed by the union of the central layer

Theorem 3.1. *Let G be a connected graph of order n with diameter D. Then*
$\xi^d(G) \geq -\frac{D+1}{96}\left[7D^3 - (32n + 23)D^2 + (44n + 1)D - 48n^2 + 36n + 15\right]$, *if D is odd;*
$\xi^d(G) \geq -\frac{D}{96}\left[7D^3 - (32n + 28)D^2 + (24n - 28)D - 48n^2 + 32n + 16\right]$, *if D is even.*
with equality holding if and only if $G \cong G_D^*$ for even D and $G \in \mathcal{G}_D^\blacklozenge$ for odd D.

Proof. Let $G_0 \in \mathcal{G}_{n,D}$ be a graph with the minimal eccentric distance sum. Let $P_{D+1} = v_0 v_1 \ldots v_D$ be the diametrical path in G_0. From Lemma 2.3, the subgraphs induced by the union of two neighboring distance layers in G_0 are complete.

Assume that $k \in \{1, \ldots, \lceil\frac{D-1}{2}\rceil - 1\}$ is the smallest number such that $|V_k| > 1$. Let v be a vertex in V_k different from v_k. We may construct a new graph G_0' from G_0 by removing v from V_k to V_{k+1} such that G_0' has the diameter D and the subgraphs induced by the union of two neighboring distance layers in G_0' are complete. From the definition, we have

$\xi^d(G_0) = \sum_{u\in V_0\cup\ldots\cup V_{k-1}} \varepsilon(u)D(u) + \sum_{u\in V_k\setminus\{v\}} \varepsilon(u)D(u) + \sum_{u\in V_{k+1}\cup\ldots\cup V_D} \varepsilon(u)D(u)$
$+ \varepsilon(v)D(v),$

$\xi^d(G_0') = \sum_{u\in V_0\cup\ldots\cup V_{k-1}} \varepsilon(u)(D(u)+1) + \sum_{u\in V_k\setminus\{v\}} \varepsilon(u)D(u) + \sum_{u\in V_{k+1}\cup\ldots\cup V_D} \varepsilon(u)(D(u)$
$- 1) + (\varepsilon(v) - 1)(D(v) + k - |V_{k+2}| - | V_{k+3}| - \ldots - |V_D|).$

Bear in mind that $k \le \lceil \frac{D-1}{2} \rceil - 1$, and $|V_i| \ge 1$ for $i = k+2, k+3, \dots, n$, therefore $k - |V_{k+2}| - |V_{k+3}| - \dots - |V_D| \le 0$. Thus it follows that

$$\begin{aligned}\xi^d(G_0) - \xi^d(G_0') &= -\sum_{u \in V_0 \cup \dots \cup V_{k-1}} \varepsilon(u) + \sum_{u \in V_{k+1} \cup \dots \cup V_D} \varepsilon(u) + D(v) \\ &\quad - (\varepsilon(v) - 1)(k - |V_{k+2}| - |V_{k+3}| - \dots - |V_D|) \\ &> -\sum_{u \in V_0 \cup \dots \cup V_{k-1}} \varepsilon(u) + \sum_{u \in V_{k+1} \cup \dots \cup V_D} \varepsilon(u) \ge 0.\end{aligned}$$

This contradicts the fact that G_0 has the minimal eccentric distance sum in $\mathcal{G}_{n,D}$.

Next, we assume that $k \in \{\lceil \frac{D+1}{2} \rceil + 1, \dots, D-1\}$ is the largest number such that $|V_k| > 1$. Let w be a vertex in V_k different to v_k. Then we may construct a new graph G_0'' from G_0 by removing w from V_k to V_{k-1} such that G_0'' has the diameter D and the subgraphs induced by the union of two neighboring distance layers in G_0'' are complete. Similar as above, we get that $\xi^d(G_0) > \xi^d(G_0'')$ and this also leads to a contradiction.

Therefore, G_D^* is the unique graphs with minimal eccentric distance sum in $\mathcal{G}_{n,D}$ for even D; it can be seen that all graphs from $\mathcal{G}_D^{\bullet}$ have the same eccentric distance sum $\xi^d(G_D^*)$ and there are exactly $\lceil \frac{n-D}{2} \rceil$ extremal graphs with minimal eccentric distance sum for odd D. □

4 Maximal Harary index of graphs

In [22] the authors obtained sharp lower bound for the Wiener index of graphs in $\mathcal{G}_{n,D}$. Since that method can not be generalized, we use a different approach to study the Harary index of graphs with given diameter.

The value $H(C_n)$ is well-known (see for example [8])

$$H(C_n) = \begin{cases} n\sum_{k=1}^{\frac{n}{2}-1} \frac{1}{k} + 1, & \text{if } n \text{ is even;} \\ n\sum_{k=1}^{\frac{n-1}{2}-1} \frac{1}{k}, & \text{if } n \text{ is odd.} \end{cases}$$

Theorem 4.1. *Let $G \in \mathcal{G}_{n,D}$ be a connected graph of order $n \ge 2$ with diameter $n-2 \ge D \ge 2$. Then $H(G) \le H(G_D^*)$. The equality holds if and only if $G \cong G_D^*$.*

Proof. If $D = 2$, since adding edges would decrease the distance of some pairs of vertices and hence increase the Harary index, in this case, the extremal graph is $K_n - e$ (obtained from the complete graph K_n by deleting one edge). Therefore in the sequel, we always assume that $D \ge 3$.

We first prove the case when D is even. Let x and y be two vertices of G at distance D. We distinguish in the following two cases.

Case 1. If x and y does not lie in a cycle, we suppose that P is a path with $D+1$ vertices connecting x and y. We label the vertices in P by $x = w_1, w_2, w_3, \ldots, w_{D+1} = y$. Let $Q = V(G) \setminus V(P)$. Note that any vertex in Q has at most three neighbors on P, and if a vertex in Q has three neighbors on P, they must be consecutive.

For any pairs of vertices $u, v \in Q$, $d(u,v) \geq 1$. The equality holds for all pairs if and only if Q induces a complete subgraph in G. Since adding edges increases the Harary index, for an arbitrary vertex $v \in Q$, we can suppose that v is adjacent to w_s, w_{s+1}, w_{s+2}. Let $t = D - s$, and

$$\begin{aligned}\sum_{u\in P} \tfrac{1}{d(u,v)} &= 1 + \left(1 + \tfrac{1}{2} + \ldots + \tfrac{1}{s}\right) + \left(1 + \tfrac{1}{2} + \ldots + \tfrac{1}{t}\right)\\ &\leq 1 + 2\left(1 + \tfrac{1}{2} + \ldots + \tfrac{1}{\frac{D}{2}}\right).\end{aligned}$$

with equality holding if and only if $s = t = \frac{D}{2}$.

Therefore it follows that

$$\begin{aligned}H(G) &= \sum_{u,v\in P} \tfrac{1}{d(u,v)} + \sum_{u,v\in Q} \tfrac{1}{d(u,v)} + \sum_{v\in Q, u\in P} \tfrac{1}{d(u,v)}\\ &\leq H(P_{D+1}) + \binom{n-D-1}{2} + (n-D-1)\left(1 + 2\sum_{k=1}^{\frac{D}{2}} \tfrac{1}{k}\right)\\ &= 1 + (D+1)\sum_{k=2}^{D} \tfrac{1}{k} + \tfrac{1}{2}(n-D-1)(n-D-2) + (n-D-1)\left(1 + 2\sum_{k=1}^{\frac{D}{2}} \tfrac{1}{k}\right)\\ &= -D + (D+1)\sum_{k=1}^{D} \tfrac{1}{k} + \tfrac{1}{2}(n-D-1)(n-D) + 2(n-D-1)\sum_{k=1}^{\frac{D}{2}} \tfrac{1}{k}\\ &= H(G_D^*),\end{aligned}$$

with equality holding if and only if $G \cong G_D^*$.

Case 2. If x and y lie in a cycle C, then C has $2D$ or $2D+1$ vertices.

Let $U = V(G) \setminus V(C)$. As in Case 1, for any pairs of vertices $u, v \in U$, $d(u,v) \geq 1$. The equality holds if and only if the subgraph induced by U is complete.

Subcase 2.1. If C has $2D$ vertices, then any vertex u in U has at most three neighbors on C. Moreover if u has three neighbors on C, they must be consecutive, or otherwise one can see that the diameter will be decreased.

For any vertex $v \in U$, we have

$$\begin{aligned}\sum_{u\in C} \tfrac{1}{d(u,v)} &\leq 1 + \left(1 + \tfrac{1}{2} + \ldots + \tfrac{1}{D}\right) + \left(1 + \tfrac{1}{2} + \ldots + \tfrac{1}{D-1}\right)\\ &= 3 + 2\sum_{k=2}^{D-1} \tfrac{1}{k} + \tfrac{1}{D}.\end{aligned}$$

Therefore, for $n \geq 2D$,

$$H(G) = \sum_{u,v\in C} \tfrac{1}{d(u,v)} + \sum_{u,v\in U} \tfrac{1}{d(u,v)} + \sum_{v\in U, u\in C} \tfrac{1}{d(u,v)}$$

$$\leq H(C_{2D}) + \binom{n-2D}{2} + (n-2D)\Big(3 + 2\sum_{k=2}^{D-1}\frac{1}{k} + \frac{1}{D}\Big)$$
$$= 2D\sum_{k=1}^{D-1}\frac{1}{k} + 1 + \frac{1}{2}(n-2D-1)(n-2D) + (n-2D)\Big(1 + 2\sum_{k=1}^{D-1}\frac{1}{k} + \frac{1}{D}\Big)$$
$$= 2(n-D)\sum_{k=1}^{D-1}\frac{1}{k} + 1 + \frac{1}{2}(n-2D-1)(n-2D) + (n-2D)(1+\frac{1}{D})$$
$$= 2(n-D)\sum_{k=1}^{D}\frac{1}{k} + 1 + \frac{1}{2}(n-2D+1)(n-2D) - \frac{n}{D}$$
$$< -D + (D+1)\sum_{k=1}^{D}\frac{1}{k} + \frac{1}{2}(n-D-1)(n-D) + 2(n-D-1)\sum_{k=1}^{\frac{D}{2}}\frac{1}{k}$$

We are now to show the last inequality holds. Let $M = \sum_{k=1}^{D}\frac{1}{k}$, $N = \sum_{k=1}^{\frac{D}{2}}\frac{1}{k} \geq \sum_{k=1}^{\frac{D}{2}}\frac{2}{D} = 1$, $T = M - N = \sum_{k=\frac{D}{2}+1}^{D}\frac{1}{k} < \sum_{k=\frac{D}{2}+1}^{D}\frac{2}{D} = 1$. Then we have

$$\Big(2(n-D)\sum_{k=1}^{D}\frac{1}{k} + 1 + \frac{1}{2}(n-2D+1)(n-2D) - \frac{n}{D}\Big)$$
$$-\Big(-D + (D+1)\sum_{k=1}^{D}\frac{1}{k} + \frac{1}{2}(n-D-1)(n-D) + 2(n-D-1)\sum_{k=1}^{\frac{D}{2}}\frac{1}{k}\Big)$$
$$= \Big(2(n-D)M + 1 + \frac{1}{2}(n-2D+1)(n-2D) - \frac{n}{D}\Big)$$
$$-\Big(-D + (D+1)M + \frac{1}{2}(n-D-1)(n-D) + 2(n-D-1)N\Big)$$
$$= (2n-3D-1)M - 2(n-D-1)N + 1 - \frac{n}{D} + D - \frac{1}{2}(2Dn - 2n - 3D^2 + 3D)$$
$$= (-D+1)N + (2n-3D-1)T + 1 - \frac{n}{D} + D - \frac{1}{2}(2Dn - 2n - 3D^2 + 3D)$$
$$< (-D+1) + (2n-3D-1) + 1 - \frac{n}{D} + D - \frac{1}{2}(2Dn - 2n - 3D^2 + 3D)$$
$$= \frac{1}{2}(2 - 9D + 3D^2 + 6n - 2Dn) - \frac{n}{D}$$
$$\leq \frac{1}{2}(2 - 9D + 3D^2 + (6-2D)2D) - 2$$
$$= -\frac{1}{2}(D-3)(D+1) - 2 < 0 \quad \text{for } D \geq 3 \text{ and } n \geq 2D.$$

Therefore, in this case, we get that $H(G) < H(G_D^*)$.

Subcase 2.2. If C has $2D+1$ vertices, by a similar reasoning as in Subcase 2.1, we conclude that $H(G) < H(G_D^*)$.

For D odd, just let $s = \frac{D+1}{2}$, $t = \frac{D-1}{2}$, and the remaining is similar. In this case

$$H(G_D^*) = \sum_{u,v\in P}\frac{1}{d(u,v)} + \sum_{u,v\in Q}\frac{1}{d(u,v)} + \sum_{v\in Q,u\in P}\frac{1}{d(u,v)}$$
$$= H(P_{D+1}) + \binom{n-D-1}{2} + (n-D-1)\Big(1 + \sum_{k=1}^{\frac{D+1}{2}}\frac{1}{k} + \sum_{k=1}^{\frac{D-1}{2}}\frac{1}{k}\Big)$$
$$= 1 + (D+1)\sum_{k=2}^{D}\frac{1}{k} + \frac{1}{2}(n-D-1)(n-D-2)$$
$$+ (n-D-1)\Big(1 + \sum_{k=1}^{\frac{D+1}{2}}\frac{1}{k} + \sum_{k=1}^{\frac{D-1}{2}}\frac{1}{k}\Big)$$
$$= -D + (D+1)\sum_{k=1}^{D}\frac{1}{k} + \frac{1}{2}(n-D-1)(n-D) + (n-D-1)\Big(\sum_{k=1}^{\frac{D+1}{2}}\frac{1}{k} + \sum_{k=1}^{\frac{D-1}{2}}\frac{1}{k}\Big).$$

Combining the above cases and the definition of $H(G)$, we get the result. □

From the proof of the above theorem, we have

$$H(G_D^*) = \begin{cases} -D + (D+1)\sum_{k=1}^{D} \frac{1}{k} + \frac{1}{2}(n-D-1)(n-D) \\ +2(n-D-1)\sum_{k=1}^{\frac{D}{2}} \frac{1}{k}, \quad \text{if } D \text{ is even;} \\ -D + (D+1)\sum_{k=1}^{D} \frac{1}{k} + \frac{1}{2}(n-D-1)(n-D) \\ +(n-D-1)\Big(\sum_{k=1}^{\frac{D+1}{2}} \frac{1}{k} + \sum_{k=1}^{\frac{D-1}{2}} \frac{1}{k}\Big), \quad \text{if } D \text{ is odd.} \end{cases}$$

5 Degree powers of graphs with fixed diameter

Lemma 5.1. *For $D = 3$, the graph G_D^* has maximal degree powers.*

Proof. Let G be the extremal graph having diameter 3. By Lemma 2.3, $n_1 + n_2 = n - 2$, $1 \le n_1 \le n - 3$, thus it follows that

$$\begin{aligned} F_p(G) &\le n_1^p + n_1(n_1+n_2)^p + n_2(n_1+n_2)^p + n_2^p \\ &= n_1^p + (n_1+n_2)^{p+1} + n_2^p \\ &= n_1^p + (n-2)^{p+1} + (n-2-n_1)^p. \end{aligned}$$

Now we consider the function $f(x) = x^p + (n-2-x)^p$, where $1 \le x \le n-3$. It is easy to check that

$$\frac{d^2 f(x)}{dx^2} = p(p-1)(x^{p-2} + (n-2-x)^{p-2}) > 0,$$

therefore the maximum value of $f(x)$ is obtained for $x = 1, n-3$.

It follows that

$$n_1^p + (n-2)^{p+1} + (n-2-n_1)^p \le 1 + (n-2)^{p+1} + (n-3)^p = F_p(G_D^*).$$

The inequality is equality if and only if $n_1 = 1$ or $n_1 = n-3$. □

Theorem 5.2. *Let $G \in \mathcal{G}_{n,D}$ be a connected graph of order n with diameter $D \ge 4$. If G has the maximal degree powers, then G is isomorphic to G_{l_1,l_2} (as shown in Fig. 1).*

Proof. Let $P = x_0x_1x_2\ldots x_{D-1}x_D$ be a diametral path with $D+1$ vertices connecting the vertices $x_0 = u$ and $x_D = v$. Let U be the set of neighbors of P outside P, i.e., $U = N(P) \setminus V(P)$, $W = V(G) \setminus \{U \cup V(P)\}$. Note that any vertex not in P has at most three neighbors on P, and if a vertex not in P has three neighbors in P, the neighbors must be consecutive. For $x \in V(P)$, let $N_U(x)$ be the neighbor set of x in U.

We now use the following operation. For any pair of vertices $x_j, x_k \in V(P)$ $(0 \le i, j \le D)$ such that $d(x_j) \ge 3$, $d(x_k) \ge 3$, if $N_U(x_j) \ne N_U(x_k)$, then we can delete edges between x_j and $N_U(x_j) \setminus N_U[x_k]$ and then add edges between x_k and $N_U(x_j) \setminus N_U[x_k]$; or delete edges between x_k and $N_U(x_k) \setminus N_U[x_j]$ and then add edges between x_j and $N_U(x_k)\setminus N_U[x_j]$. Then the number of vertices in P of degree at least three decreases. From Lemma 2.2, this operation increases $F_p(G)$ while keeping P fixed.

By performing the above operation several times, we finally get a graph H with diametral path P without two vertices $x_j, x_k \in V(P)$ such that $d(x_j) \geq 3$, $d(x_k) \geq 3$ and $d_P(x_j, x_k) \geq 4$. That is, there are at most three vertices in P having degree at least 3. Now adding all possible edges between vertices in $V(G) \setminus V(P)$, the value F_p increases, and we get the extremal graph is G_{l_1,l_2}.

From the above cases, we complete the proof. □

For $D \geq 4$, we have

$$F_p(G_{l_1,l_2}) = (n-D+2)(n-D+1)^p + (D-4)2^p + 2.$$

Finally we summarize the results of this section.

Theorem 5.3. *Let $G \in \mathcal{G}_{n,D}$ be a connected graph of order $n \geq 3$ with diameter $3 \leq D \leq n-2$ and maximal degree powers. Then G must be of the form G_{l_1,l_2} and furthermore*

(1) If $D = 3$, then $l_1 = 1$, $l_2 = 0$;

(2) If $D = 4$, then $l_1 = l_2 = 1$;

(3) If $D = 5$, then $l_1 = 2$, $l_2 = 1$;

(4) If $D \geq 6$, then $l_1 \geq 2$, $l_2 \geq 2$.

Remark. Li and Zheng [21] defined the so called *zeroth-order general Randić index* $R^0_\alpha(G)$ of a graph G as

$$R^0_\alpha(G) = \sum_{v\in V(G)} d(u)^\alpha$$

for general real number α.

In fact, the result in Theorem 5.3 holds for any positive real number α of $R^0_\alpha(G)$.

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