

# Minimal energy of unicyclic graphs of a given diameter

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The energy of a graph is defined as the sum of the absolute values of all the eigenvalues of the graph. For a given positive integer  $d$  with  $3 \leq d \leq n - 2$ , we characterize the graphs with minimal energy in the class of unicyclic graphs with  $n$  vertices and a given diameter  $d$ .

**KEY WORDS:** energy, diameter, unicyclic graphs, characteristic polynomial

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## 1. Introduction

Let  $G$  be a simple graph with  $n$  vertices. The characteristic polynomial of  $G$ , denoted by  $\phi(G)$ , is defined as

$$\phi(G) = \det(xI - A(G)) = \sum_{i=0}^n a_i(G)x^{n-i},$$

where  $I$  is the identity matrix of order  $n$  and  $A(G)$  is an adjacency matrix of  $G$ . The roots of the equation  $\phi(G) = 0$ , denoted by  $\lambda_1, \lambda_2, \dots, \lambda_n$ , are the eigenvalues of the graph  $G$ . Since  $A(G)$  is symmetric, all eigenvalues of  $G$  are real. The energy of  $G$ , denoted by  $E(G)$ , is then defined by

$$E(G) = \sum_{i=1}^n |\lambda_i|.$$

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In chemistry, the energy of a given molecular graph is of interest since it is closely related to the total  $\pi$ -electron energy of the molecule represented by that graph. See Refs. [1–3] for more details on graph-energy concept and a survey of the mathematical properties and results.

For a graph  $G$  with  $n$  vertices, let  $b_i(G) = |a_i(G)|$ ,  $i = 0, 1, \dots, n$ . Note that  $b_0(G) = 1$ ,  $b_1(G) = 0$ , and  $b_2(G)$  is the number of edges of  $G$ . For convenience, let  $b_i(G) = 0$  if  $i < 0$ . Let  $m(G, k)$  be number of  $k$ -matchings of  $G$ . If  $G$  is an acyclic graph, then [1]  $b_{2k}(G) = m(G, k)$  and  $b_{2k+1}(G) = 0$  for all  $k$ .

A connected graph with  $n$  vertices and  $n$  edges is called a unicyclic graph. Obviously, a unicyclic graph has exactly one cycle.

Let  $\mathcal{G}(n)$  be the class of graphs with  $n$  vertices whose components are all trees except at most one being a unicyclic graph. That is, any graph in  $\mathcal{G}(n)$  is either acyclic or contains exactly one cycle. By Sachs theorem and the Coulson integral formula [1, 2], we have [4, 5]

$$E(G) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{dx}{x^2} \ln \left[ \left( \sum_{j=0}^{\lfloor n/2 \rfloor} b_{2j}(G)x^{2j} \right)^2 + \left( \sum_{j=0}^{\lfloor n/2 \rfloor} b_{2j+1}(G)x^{2j+1} \right)^2 \right]. \quad (1)$$

Thus  $E(G)$  is a monotonically increasing function of  $b_i(G)$ ,  $i = 1, 2, \dots, n$ . Let  $G_1, G_2 \in \mathcal{G}(n)$ . If  $b_i(G_1) \geq b_i(G_2)$  for all  $i \geq 0$ , then we write  $G_1 \succeq G_2$ . If  $G_1 \succeq G_2$  and there is an  $i_0$  such that  $b_{i_0}(G_1) > b_{i_0}(G_2)$ , then we write  $G_1 > G_2$ . So from (1) we have the following increasing property of energy:

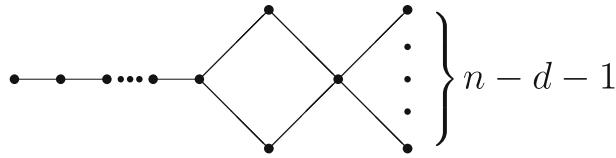
$$G_1 > G_2 \Rightarrow E(G_1) > E(G_2). \quad (2)$$

This increasing property of energy has been used in the study of extremal values of energy over some classes of graphs. For instance, Gutman [4] determined the trees with minimal and maximal energies. Hou [5] determined the unicyclic graphs with minimal energy, and Yan and Ye [6] determined trees of a given diameter with minimal energy. More results in this direction can be found in Refs. [7–12].

Let  $\mathcal{U}(n, d)$  be the class of unicyclic graphs with  $n$  vertices and diameter  $d$ , where  $2 \leq d \leq n - 2$ . By the result of Ref. [5], the graph obtained by attaching  $n - 3$  pendant edges to a vertex of a triangle is the unique graph in  $\mathcal{U}(n, 2)$  with minimal energy. In this paper, we will prove that for  $3 \leq d \leq n - 2$ , the graph  $U_{n,d}$  is the unique graph in  $\mathcal{U}(n, d)$  with minimal energy, where the graph  $U_{n,d}$  is shown in figure 1.

## 2. Preliminaries

Denote by  $P_n$  the path with  $n$  vertices. For two graphs  $G$  and  $H$ ,  $G \neq H$  means  $G$  and  $H$  are not isomorphic, and  $G \supseteq H$  means  $G$  contains  $H$  as a subgraph.

Figure 1. Graph  $U_{n,d}$  with  $d \geq 3$ .

**Lemma 1.** Let  $G$  be a graph in  $\mathcal{G}(n)$ .

(a) If  $G$  contains exactly one cycle  $C_r$  and  $uv$  is an edge on this cycle, then

$$\begin{aligned} b_i(G) &= b_i(G - uv) + b_{i-2}(G - u - v) - 2b_{i-r}(G - C_r) \text{ if } r \equiv 0 \pmod{4}, \\ b_i(G) &= b_i(G - uv) + b_{i-2}(G - u - v) + 2b_{i-r}(G - C_r) \text{ if } r \not\equiv 0 \pmod{4}. \end{aligned}$$

(b) If  $uv$  is a cut edge of  $G$ , then

$$b_i(G) = b_i(G - uv) + b_{i-2}(G - u - v).$$

*Proof.* For edge  $uv$  of  $G$ , it is known [1, 13] that

$$\phi(G) = \phi(G - uv) - \phi(G - u - v) - 2 \sum_{C \in \mathcal{C}} \phi(G - C),$$

where  $\mathcal{C}$  is the set of cycles of  $G$  containing  $uv$ . In particular, if  $uv$  is a cut edge, then

$$\phi(G) = \phi(G - uv) - \phi(G - u - v).$$

Now (a) and (b) follow by equating coefficients of  $x^{n-2k}$  on both sides of identities above.  $\square$

*Remark.* If  $uv$  is a pendant edge with pendant vertex  $u$ , then lemma 1(b) becomes

$$b_i(G) = b_i(G - u) + b_{i-2}(G - u - v).$$

**Lemma 2.** Let  $G$  be an acyclic graph and  $G'$  a spanning subgraph (resp. proper spanning subgraph) of  $G$ . Then  $G \succeq G'$  (resp.  $\succ G'$ ).

**Lemma 3.** Let  $G$  be a unicyclic graph and  $G'$  a graph obtained from  $G$  by deleting at least one edge outside its unique cycle. Then  $G \succ G'$ .

*Proof.* Let  $H \in \{G, G'\}$  and  $uv$  be an edge on the unique cycle  $C_r$  in  $H$ .

If  $r \not\equiv 0 \pmod{4}$ , by lemma 1 (a)

$$b_i(H) = b_i(H - uv) + b_{i-2}(H - u - v) + 2b_{i-r}(H - C_r).$$

Since  $G'$  is a proper spanning subgraph of  $G$ , we have by lemma 2 that  $b_i(G - uv) \geq b_i(G' - uv)$ ,  $b_{i-2}(G - u - v) \geq b_{i-2}(G' - u - v)$ , and  $b_{i-r}(G - C_r) \geq b_{i-r}(G' - C_r)$ . So we have  $b_i(G) \geq b_i(G')$ , and  $b_2(G) > b_2(G')$ , and then  $G \succ G'$ .

If  $r \equiv 0 \pmod{4}$ , then  $b_{2k+1}(H) = 0$ . By lemma 1 (a)

$$\begin{aligned} b_{2k}(H) &= b_{2k}(H - uv) + b_{2k-2}(H - u - v) - 2b_{2k-r}(H - C_r) \\ &= m(H, k) - 2m(H - C_r, k - \frac{r}{2}), \end{aligned}$$

i.e.,  $b_{2k}(H)$  is the number of  $k$ -matchings of  $H$  that contain at most  $r/2 - 1$  edges of the cycle  $C_r$ . So  $b_{2k}(H) = \sum_S m(H_S, k - |S|)$ , where summation goes over all non-perfect matchings  $S$  of  $C_r$ , and where  $H_S$  is the graph obtained from  $H$  by deleting the end vertices of  $S$  and other edges of  $C_r$ . Since for any  $S$ ,  $G'_S$  is a subgraph of  $G_S$ , we have  $m(G_S, k - |S|) \geq m(G'_S, k - |S|)$  and then  $b_{2k}(G) \geq b_{2k}(G')$  for all  $k$ . Note that  $b_2(G) > b_2(G')$ . We have  $G \succ G'$ .  $\square$

**Lemma 4.** [1, 12]. For  $2 \leq i \leq \lfloor \frac{n}{2} \rfloor$  and  $n \geq 4$ ,

$$P_n \succ P_i \cup P_{n-i} \succ P_1 \cup P_{n-1}.$$

Let  $T(n, d)$  be the class of trees with  $n$  vertices and diameter  $d$ , where  $2 \leq d \leq n - 2$ . Let  $B_{n,d}$  be a graph obtained from the path  $P_d$  by attaching  $n - d$  pendant edges to an end vertex of  $P_d$ . Let  $Y_n = B_{n,3}$ . Let  $K_{1,n-1}$  be the star with  $n$  vertices.

**Lemma 5.** [4]. For  $n \geq 5$ ,

$$P_n \succ Y_n \succ K_{1,n-1}.$$

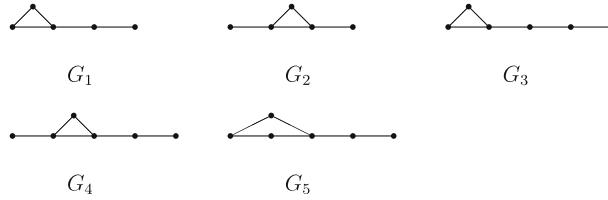
**Lemma 6.** [6]. Let  $T \in T(n, d)$  and  $T \neq B_{n,d}$ . Then  $T \succ B_{n,d}$ .

**Lemma 7.** If  $d > d_0 \geq 3$ , then  $B_{n,d} \succ B_{n,d_0}$ .

*Proof.* Note that for any integer  $k \geq 1$ ,

$$\begin{aligned} m(B_{n,d}, k) &= m(B_{n-1,d-1}, k) + m(B_{n-2,d-2}, k - 1), \\ m(B_{n,d-1}, k) &= m(B_{n-1,d-1}, k) + m(P_{d-2}, k - 1). \end{aligned}$$

Since  $P_{d-2}$  is a proper subgraph of  $B_{n-2,d-2}$ , we have  $m(B_{n-2,d-2}, k - 1) \geq m(P_{d-2}, k - 1)$  and this inequality strict for  $k = 2$ . Hence  $m(B_{n,d}, k) \geq m(B_{n,d-1}, k)$  and this inequality strict for  $k = 2$ . It follows that  $B_{n,d} \succ B_{n,d-1} \succ \dots \succ B_{n,d_0}$ .  $\square$

Figure 2. Graphs  $G_i$ ,  $i = 1, \dots, 5$ .

For minimal energies in  $\mathcal{T}(n, d)$ , we point out that in [12, theorem 1] a condition  $T \neq T(n, d; 1, 0, \dots, 0, n - d - 2)$  should be added.

By lemma 1 (b), it is easy to see that the following lemma holds. It is known [9] that similar result holds for bipartite graphs.

**Lemma 8.** Let  $G, G' \in \mathcal{G}(n)$ . Let  $uv$  (resp.  $u'v'$ ) be a pendant edge with the pendant vertex  $u$  (resp.  $u'$ ) of the graph  $G$  (resp.  $G'$ ). If  $G - u \succeq G' - u'$ , and  $G - u - v \succ G' - u' - v'$ , or  $G - u \succ G' - u'$ , and  $G - u - v \succeq G' - u' - v'$ , then  $G \succ G'$ .

### 3. Main results

Now we consider the minimal energy of graphs in  $\mathcal{U}(n, d)$  with  $3 \leq d \leq n - 2$ . We first consider the case  $d = n - 2$ .

**Lemma 9.** Let  $G \in \mathcal{U}(n, n - 2)$  with  $n \geq 5$  and  $G \neq U_{n,n-2}$ . Then  $G \succ U_{n,n-2}$ .

*Proof.* We prove the lemma by induction on  $n$ .

If  $n = 5$ , then  $G$  is isomorphic to  $G_1$  or  $G_2$ . (See figure 2.) It is easy to see that

$$\begin{aligned} \phi(G_1) &= x^5 - 5x^3 - 2x^2 + 4x + 2, & \phi(G_2) &= x^5 - 5x^3 - 2x^2 + 3x, \\ \phi(U_{5,3}) &= x^5 - 5x^3 + 2x. \end{aligned}$$

It is obvious that  $G_i \succ U_{5,3}$  for  $i = 1, 2$ .

If  $n = 6$ , then  $G$  is isomorphic to  $G_3$ ,  $G_4$  or  $G_5$ . (See figure 2.) Note that

$$\begin{aligned} \phi(G_3) &= x^6 - 6x^4 - 2x^3 + 8x^2 + 4x - 1, & \phi(G_5) &= x^6 - 6x^4 + 6x^2, \\ \phi(G_4) &= x^6 - 6x^4 - 2x^3 + 7x^2 + 2x - 1, & \phi(U_{6,4}) &= x^6 - 6x^4 + 5x^2. \end{aligned}$$

It is obvious that  $G_i \succ U_{6,4}$  for  $i = 3, 4, 5$ .

Suppose that the result holds for graphs in  $\mathcal{U}(n-1, n-3)$  and  $\mathcal{U}(n-2, n-4)$  and that  $G \in \mathcal{U}(n, n-2)$  and  $G \neq U_{n,n-2}$  where  $n \geq 7$ .

Let  $u$  (resp.  $u'$ ) be a pendant vertex, adjacent to  $v$  (resp.  $v'$ ), which has the largest distance to a vertex on the unique cycle of  $G$  (resp.  $U_{n,n-2}$ ). Then the degree of  $v$  is 2. So  $G - u \in \mathcal{U}(n-1, n-3)$ ,  $G - u - v \in \mathcal{U}(n-2, n-4)$ , and  $U_{n,n-2} - u' = U_{n-1,n-3}$ ,  $U_{n,n-2} - u' - v' = U_{n-2,n-4}$ .

Since  $G \neq U_{n,n-2}$ , we have  $G - u \neq U_{n-1,n-3}$  or  $G - u - v \neq U_{n-2,n-4}$ . By the induction assumption, we have either  $G - u \succ U_{n-1,n-3}$  and  $G - u - v \succeq U_{n-2,n-4}$ , or  $G - u \succeq U_{n-1,n-3}$  and  $G - u - v \succ U_{n-2,n-4}$ . By lemma 8,  $G \succ U_{n,n-2}$ .  $\square$

Now we are ready to prove our main result:

**Theorem 1.** Let  $G \in \mathcal{U}(n, d)$  with  $d \geq 3$  and  $G \neq U_{n,d}$ . Then  $E(G) > E(U_{n,d})$ .

*Proof.* By the increasing property (2) of energy, it suffices to prove that  $G \succ U_{n,d}$ . We prove this by induction on  $n - d$ .

By lemma 9, the result holds for  $n - d = 2$ .

Let  $p \geq 3$  and suppose that the result holds for  $n - d < p$ . Now suppose that  $n - d = p$ . Let  $u'$  be the vertex of degree 3 in  $U_{n,d}$  and  $v'$  a vertex on the quadrangle that is adjacent to  $u'$ . By lemma 1 (a)

$$b_i(U_{n,d}) = b_i(B_{n,d}) + b_{i-2}(P_{d-3} \cup K_{1,n-d}) - 2b_{i-4}(P_{d-3}).$$

First note that  $b_n(C_n) \geq 0 = b_n(U_{n,d})$ , and that if  $0 \leq i \leq n - 1$ , then by lemma 1 (a)

$$b_i(C_n) = b_i(P_n) + b_{i-2}(P_{n-2}).$$

By lemma 7,  $P_n \succ B_{n,d}$  and by lemma 4,  $P_{n-2} \succeq P_{d-3} \cup P_{n-d+1} \succ P_{d-3} \cup K_{1,n-d}$ . So  $b_i(C_n) \geq b_i(U_{n,d})$  and  $b_4(C_n) > b_4(U_{n,d})$ . Thus  $C_n \succ U_{n,d}$ .

In the following, suppose that the unique cycle of  $G$  is  $C_r$  where  $r < n$ . Let  $P(G) = v_0, v_1, \dots, v_d$  be a diametrical path of  $G$ . Then one of  $v_0, v_d$  must be a pendant vertex.

Suppose that all pendant vertices are on  $P(G)$ . Since  $p \geq 3$ , there are at least two adjacency vertices  $u$  and  $v$  on  $C_r$  which are outside  $P(G)$  such that  $G - uv \in \mathcal{T}(n, d_1)$ ,  $G - v \in \mathcal{T}(n - 1, d_2)$  and  $G - u - v \in \mathcal{T}(n - 2, d_3)$ , where  $d_1, d_2, d_3 \geq d$ . By lemmas 6 and 7,  $G - uv \succeq B_{n,d_1} \succeq B_{n,d}$ ,  $G - v \succeq B_{n-1,d_2} \succeq B_{n-1,d}$ , and  $G - u - v \succeq B_{n-2,d_3} \succeq B_{n-2,d}$ .

If  $r \not\equiv 0 \pmod{4}$ , then

$$b_i(G) = b_i(G - uv) + b_{i-2}(G - u - v) + 2b_{i-r}(G - C_r).$$

By lemmas 2 and 5,  $G - u - v \succeq B_{n-2,d} \succ P_{d-3} \cup Y_{n-d-1} \succ P_{d-3} \cup K_{1,n-d}$ . Then  $b_i(G) \geq b_i(U_{n,d})$  and  $b_r(G) > b_r(U_{n,d})$ . Thus  $G \succ U_{n,d}$ .

If  $r \equiv 0 \pmod{4}$ , then by lemma 1 (a), the expression for  $b_i(U_{n,d})$  above may be written as

$$b_i(U_{n,d}) = b_i(B_{n-1,d}) + b_{i-2}(P_{d-2}) + b_{i-2}(P_{d-3} \cup K_{1,n-d-1}).$$

Suppose that  $r \neq 4$ . Then  $u$  and  $v$  can be chosen such that there is a vertex  $w$  on  $C_r$  but outside  $P(G)$ ,  $v$  is adjacent to  $u$  and  $w$ , and  $G - u - v - w \in$

$T(n-3, d_4)$  with  $d_4 \geq d$ . By lemmas 6 and 7,  $G - u - v - w \succeq B_{n-3, d_4} \succeq B_{n-3, d}$ . Let  $u_1$  (resp.  $w_1$ ) be the vertex adjacent to  $u$  (resp.  $w$ ) in  $C_r$  and  $u_1 \neq v$  (resp.  $w_1 \neq v$ ). By lemma 1 (b),  $b_{i-4}(G - u_1 - u - v - w) \geq b_{i-r}(G - C_r)$ ,  $b_{i-4}(G - u - v - w - w_1) \geq b_{i-r}(G - C_r)$ , and then

$$\begin{aligned} b_i(G - uv) &= b_i(G - v) + b_{i-2}(G - v - w) \\ &= b_i(G - v) + b_{i-2}(G - u - v - w) \\ &\quad + b_{i-4}(G - u_1 - u - v - w) \\ &\geq b_i(G - v) + b_{i-2}(G - u - v - w) + b_{i-r}(G - C_r), \\ b_{i-2}(G - u - v) &= b_{i-2}(G - u - v - w) + b_{i-4}(G - u - v - w - w_1) \\ &\geq b_{i-2}(G - u - v - w) + b_{i-r}(G - C_r). \end{aligned}$$

So by lemma 1 (a)

$$\begin{aligned} b_i(G) &= b_i(G - uv) + b_{i-2}(G - u - v) - 2b_{i-r}(G - C_r) \\ &\geq b_i(G - v) + 2b_{i-2}(G - u - v - w) \\ &\geq b_i(B_{n-1, d}) + 2b_{i-2}(B_{n-3, d}). \end{aligned}$$

By lemmas 2 and 5,  $B_{n-3, d} \succeq P_{d-3} \cup Y_{n-d} \succ P_{d-3} \cup K_{1, n-d-1}$ . Then  $b_{i-2}(B_{n-3, d}) \geq b_{i-2}(P_{d-3} \cup K_{1, n-d-1})$ . Note that  $b_{i-2}(B_{n-3, d}) \geq b_{i-2}(P_{d-2})$  and  $b_2(B_{n-3, d}) > b_2(P_{d-2})$ . So  $b_i(G) \geq b_i(U_{n, d})$  and  $b_4(G) > b_4(U_{n, d})$ . Thus  $G \succ U_{n, d}$ .

Suppose that  $r = 4$ . If all edges on the cycle are not on  $P(G)$ , then by a similar reasoning as above, we have  $G \succ U_{n, d}$ . Otherwise, there is exactly one edge on both  $C_4$  and  $P(G)$ . Then  $n = d + 3$ , and by lemmas 1 and 4, for some  $j$ ,  $1 \leq j \leq d - 1$ , we have

$$\begin{aligned} b_i(G) &= b_i(G - uv) + b_{i-2}(G - u - v) - 2b_{i-4}(G - C_4) \\ &= b_i(G - v) + b_{i-2}(P_j \cup P_{d+1-j}) + b_{i-2}(P_{d+1}) - 2b_{i-4}(P_j \cup P_{d-1-j}) \\ &= b_i(G - v) + b_{i-2}(P_j \cup P_{d-j}) + b_{i-4}(P_j \cup P_{d-j-1}) \\ &\quad + b_{i-2}(P_d) + b_{i-4}(P_{d-1}) - 2b_{i-4}(P_j \cup P_{d-1-j}) \\ &\geq b_i(G - v) + b_{i-2}(P_j \cup P_{d-j}) + b_{i-2}(P_d) \\ &\geq b_i(B_{n-1, d}) + b_{i-2}(P_j \cup P_{d-j}) + b_{i-2}(P_d). \end{aligned}$$

By lemma 4,  $P_j \cup P_{d-j} \succeq P_1 \cup P_{d-1} \succ 2P_1 \cup P_{d-2}$  and  $P_d \succeq P_{d-3} \cup P_3$ . Then  $b_i(G) \geq b_i(U_{n, d})$ . Since  $b_2(P_d) > b_2(P_{d-3} \cup P_3)$ , we have  $b_4(G) > b_4(U_{n, d})$ . Thus  $G \succ U_{n, d}$ .

Now suppose that there is at least one pendant vertex outside  $P(G)$ . Let  $u'$  be a pendant vertex of  $U_{n, d}$  adjacent to the vertex  $v'$  of degree  $n - d + 1$ . Then  $U_{n, d} - u' = U_{n-1, d}$  and  $U_{n, d} - u' - v' = (n - d - 2)P_1 \cup B_{d, d-2}$ .

**Case 1.** There is a pendant vertex  $u$  outside  $P(G)$  such that its neighbor  $v$  lies on  $C_r$ . Then  $G - u \in \mathcal{U}(n - 1, d)$ .

If  $v$  lies outside  $P(G)$ , then  $G - u - v \succeq P_{d+1}$ . So  $G - u - v \succeq (n - d - 3)P_1 \cup P_{d+1} \succ (n - d - 2)P_1 \cup B_{d, d-2}$ .

Suppose that  $v$  is on  $P(G)$ . Then  $P(G)$  and  $C_r$  have common vertices, say  $v_l, \dots, v_{l+s}$  with  $s \geq 0$ .

If  $s = 0$ , i.e.,  $v = v_l$  is the unique common vertex of  $P(G)$  and the cycle  $C_r$ , then  $G - u - v \supseteq P_l \cup P_{d-l} \cup P_2$ , and since

$$\begin{aligned} b_i(P_l \cup P_{d-l} \cup P_2) &= b_i(P_l \cup P_{d-l}) + b_{i-2}(P_l \cup P_{d-l}) \\ &\geq b_i(P_{d-1}) + b_{i-2}(P_{d-3}) = b_i(B_{d,d-2}) \end{aligned}$$

and  $b_4(P_l \cup P_{d-l} \cup P_2) > b_4(B_{d,d-2})$ , we have  $G - u - v \succeq (n-d-4)P_1 \cup P_l \cup P_{d-l} \cup P_2 \succ (n-d-2)P_1 \cup B_{d,d-2}$ .

Suppose that  $s > 0$ . If  $v \neq v_l, v_{l+s}$ , then  $G - u - v \supseteq P_{d+1}$ . So  $G - u - v \succeq P_{d+1} \succ P_1 \cup B_{d,d-2}$ . Otherwise, for  $j = l$  or  $l+s$ , say  $j = l$ ,  $G - u - v \supseteq P_j \cup T_1$ , where  $T_1$  obtained by attaching a pendant edge to vertex  $v_{j+s}$  of the path  $v_{j+1}, \dots, v_d$ . Note that

$$\begin{aligned} b_i(P_j \cup T_1) &= b_i(P_j \cup P_{d-j}) + b_{i-2}(P_j \cup P_{s-1} \cup P_{d-j-s}) \\ &\geq b_i(P_{d-1}) + b_{i-2}(P_{d-3}) = b_i(B_{d,d-2}). \end{aligned}$$

If  $(j, s) \neq (1, 2)$ , then  $b_6(P_j \cup T_1) > b_6(B_{d,d-2})$ , otherwise  $P_j \cup T_1$  is a proper subgraph of  $G - u - v$ . Hence we have  $G - u - v \succ (n-d-2)P_1 \cup B_{d,d-2}$ .

Now we have proved that  $G - u - v \succ U_{n,d} - u' - v'$ . By the induction hypothesis,  $G - u \succeq U_{n-1,d}$ . By lemma 8,  $G \succ U_{n,d}$ .

**Case 2.** The neighbor of any pendant vertex outside  $P(G)$  also lies outside  $C_r$ . If there is a pendant vertex  $u$ , adjacent to a vertex  $v$  outside  $P(G)$ . Then  $G - u - v \supseteq C_r \cup P_{d+1}$  or  $G - u - v \supseteq G'$  where  $G' \in \mathcal{U}(s, d)$ ,  $d+2 \leq s \leq n-2$ . If every pendant vertex outside  $P(G)$  is adjacent a vertex on  $P(G)$ , then we choose a pendant vertex  $u$ , adjacent to  $v = v_j$ , such that  $G - u - v \supseteq C_r \cup P_j \cup P_{d-j}$  or  $G - u - v \supseteq P_j \cup G''$ , where  $G'' \in \mathcal{U}(s, d')$  for some  $s$  and  $d'$  with  $s+j \leq n-2$  and  $d' \geq d-j-1$ . Hence there are three possibilities:  $G - u - v \supseteq C_r \cup P_j \cup P_{d-j}$ ,  $G - u - v \supseteq G'$  or  $G - u - v \supseteq P_j \cup G''$ .

First suppose that  $G - u - v \supseteq C_r \cup P_j \cup P_{d-j}$ . Then by lemma 1 (a)

$$\begin{aligned} b_i(C_r \cup P_j \cup P_{d-j}) &\geq b_i(P_r \cup P_j \cup P_{d-j}) + b_{i-2}(P_{r-2} \cup P_j \cup P_{d-j}) \\ &\quad - 2b_{i-r}(P_j \cup P_{d-j}) \\ &\geq b_i(P_{r-1} \cup P_j \cup P_{d-j}) + b_{i-2}(P_{r-3} \cup P_j \cup P_{d-j}) \\ &\geq b_i(P_{r-1} \cup P_{d-1}) \geq b_i(P_{d+r-3}) \geq b_i(B_{d,d-2}). \end{aligned}$$

By lemma 3,  $G - u - v \succeq (n-d-r-2)P_1 \cup C_r \cup P_j \cup P_{d-j} \succ (n-d-2)P_1 \cup B_{d,d-2}$ .

Now suppose that  $G - u - v \supseteq G'$ . By lemma 3 and the induction hypothesis,  $G - u - v \succeq (n-s-2)P_1 \cup U_{s,d} \succeq (n-d-2)P_1 \cup U_{d+2,d}$ . By lemma 1

$$\begin{aligned} b_i(U_{d+2,d}) &= b_i(B_{d+2,d}) + b_{i-2}(P_{d-3} \cup P_3) - 2b_{i-4}(P_{d-3}) \\ &= b_i(B_{d+2,d}) + b_{i-2}(P_{d-3}) \geq b_i(B_{d,d-2}). \end{aligned}$$

where  $b_2(U_{d+2,d}) > b_2(B_{d,d-2})$ . So  $G - u - v \succeq (n - d - 2)P_1 \cup U_{d+2,d} \succ (n - d - 2)P_1 \cup B_{d,d-2}$ .

Finally suppose that  $G - u - v \supseteq P_j \cup G''$ . By lemma 3 and the induction hypothesis,  $G - u - v \succeq (n - 3 - d + j)P_1 \cup U_{d-j+1,d-j-1}$ . Note that

$$\begin{aligned} b_i(P_j \cup U_{d-j+1,d-j-1}) &= b_i(P_j \cup B_{d-j+1,d-j-1}) + b_{i-2}(P_j \cup P_3 \cup P_{d-j-4}) \\ &\quad - 2b_{i-4}(P_j \cup P_{d-j-4}) \\ &= b_i(P_j \cup P_{d-j}) + b_{i-2}(P_j \cup P_{d-j-2}) \\ &\quad + b_{i-2}(P_j \cup P_{d-j-4}) \\ &\geq b_i(P_{d-1}) + b_{i-2}(P_{d-3}) = b_i(B_{d,d-2}) \end{aligned}$$

and  $b_2(P_j \cup U_{d-j+1,d-j-1}) > b_2(B_{d,d-2})$ . We have  $G - u - v \succ (n - d - 2)P_1 \cup B_{d,d-2}$ .

Now we have proved that  $G - u - v \succ U_{n,d} - u' - v'$ . By the induction hypothesis,  $G - u \succeq U_{n-1,d}$ . By lemma 8,  $G \succ U_{n,d}$ .

Combining Cases 1 and 2, we conclude that the result holds for  $G \in \mathcal{U}(n, d)$  for  $d \geq 3$ . The theorem is thus proved.  $\square$

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