# Matching Energy of Unicyclic and Bicyclic Graphs with a Given Diameter

Lin Chen, Jinfeng Liu, Yongtang Shi<sup>1</sup>

Center for Combinatorics and LPMC-TJKLC, Nankai University, Tianjin 300071, P.R. China

E-mails: chenlin1120120012@126.com, ljinfeng709@163.com, shi@nankai.edu.cn

#### Abstract

Gutman and Wagner proposed the concept of matching energy (ME) and pointed out that the chemical applications of ME go back to the 1970s. Let G be a simple graph of order n and  $\mu_1, \mu_2, \ldots, \mu_n$  be the roots of its matching polynomial. The matching energy of G is defined to be the sum of the absolute values of  $\mu_i$   $(i = 1, 2, \ldots, n)$ . In this paper, we characterize the graphs with minimal matching energy among all unicyclic and bicyclic graphs with a given diameter d.

Key words: graph; matching energy; energy; diameter

#### 1 Introduction

In this paper, all graphs under our consideration are finite, connected, undirected and simple. For more notations and terminology that will be used in the sequel, we refer to [2]. Let G be a simple undirected graph with order n and A(G) be the adjacency matrix of G. 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. The roots of the equation  $\phi(G) = 0$ , denoted by  $\lambda_1, \lambda_2, \ldots, \lambda_n$ , are the eigenvalues of A(G). The energy of

<sup>&</sup>lt;sup>1</sup>The corresponding author.

G, denoted by E(G), is defined as the sum of the absolute values of the eigenvalues of A(G), that is,

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

The concept of the energy of simple undirected graphs was introduced by Gutman in [15] and now is well-studied. For more results about graph energy, we refer the readers to recent papers [8, 9, 12, 32, 34], two surveys [16, 17] and the book [31]. There are various generalizations of graph energy, such as Randić energy [3, 10], Laplacian energy [7], distance energy [36], incidence energy [4, 5], energy of matrices [14] and energy of a polynomial [33], etc.

Let G be a simple graph with n vertices and m edges. Denote by  $m_k(G)$  the number of k-matchings(= the number of selections of k independent edges = the number of k-element independent edge sets) of G. Specifically,  $m_1(G) = m$  and  $m_k(G) = 0$  for  $k > \lfloor \frac{n}{2} \rfloor$  or k < 0. It is both consistent and convenient to define  $m_0(G) = 1$ . The matching polynomial of the graph G is defined as

$$\alpha(G) = \alpha(G, \mu) = \sum_{k>0} (-1)^k m_k(G) \mu^{n-2k}.$$
 (1)

Recently, Gutman and Wagner [23] defined the matching energy of a graph G based on the zeros of its matching polynomial [13, 21].

**Definition 1.1** Let G be a simple graph with order n, and  $\mu_1, \mu_2, \ldots, \mu_n$  be the zeros of its matching polynomial. Then,

$$ME(G) = \sum_{i=1}^{n} |\mu_i|. \tag{2}$$

Moreover, Gutman and Wagner [23] pointed out that the matching energy is a quantity of relevance for chemical applications. They arrived at the simple relation:

$$TRE(G) = E(G) - ME(G),$$

where TRE(G) is the so-called "topological resonance energy" of G. About the chemical applications of matching energy, for more details see [18, 1, 20].

For the coefficients  $a_i(G)$  of  $\phi(G)$ , let  $b_i(G) = |a_i(G)|, i = 0, 1, ..., n$ . 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. In [19, 24], we have

$$E(G) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{dx}{x^2} \ln \left[ \left( \sum_{j=0}^{\lfloor \frac{n}{2} \rfloor} b_{2j}(G) x^{2j} \right)^2 + \left( \sum_{j=0}^{\lfloor \frac{n}{2} \rfloor} b_{2j+1}(G) x^{2j+1} \right)^2 \right].$$
 (3)

Thus E(G) is a monotonically increasing function of  $b_i(G)$ , i = 0, 1, ..., n.

Being similar to Eq.(3), the matching energy also has a beautiful formula as follows[23]. Eq.(4) could be considered as the definition of matching energy, in which case Eq.(2) would become a theorem.

**Theorem 1.1** Let G be a simple graph of order n, and  $m_k(G)$  be the number of its k-matchings,  $k = 0, 1, 2, \ldots, \lfloor \frac{n}{2} \rfloor$ . The matching energy of G is given by

$$ME = ME(G) = \frac{2}{\pi} \int_0^\infty \frac{1}{x^2} \ln\left[\sum_{k>0} m_k(G) x^{2k}\right] dx.$$
 (4)

By Eq.(4) and the monotony of the function logarithm, we can define a quasi-order " $\succeq$ " as follows: If two graphs  $G_1$  and  $G_2$  have the same order and size, then

$$G_1 \succeq G_2 \iff m_k(G_1) \geq m_k(G_2)$$
 for all  $k$ .

If  $G_1 \succeq G_2$  and there exists some k such that  $m_k(G_1) > m_k(G_2)$ , then we write  $G_1 \succ G_2$ . Clearly,  $G_1 \succ G_2 \Longrightarrow ME(G_1) > ME(G_2)$ .

Notice that when  $ME(G_1) > ME(G_2)$ , we may not deduce that  $G_1 \succ G_2$ . However, if G is any simple connected graph with n vertices other than  $S_n$ , where  $S_n$  is a star of order n, then not only  $ME(G) > ME(S_n)$  [23] but also  $G \succ S_n$ . Based on the quasi-order, there are some more extremal results on matching energy of graphs [6, 26, 27, 30].

In this paper, we characterize the graphs with minimal matching energy among all unicyclic and bicyclic graphs with a given diameter d.

### 2 Preliminaries

The following result gives two fundamental identities for the number of k-matchings of a graph (see [13, 21]).

**Lemma 2.1** Let G be a simple graph, e = uv be an edge of G, and  $N(u) = \{v_1(=v), v_2, \ldots, v_j\}$  be the set of all neighbors of u in G. Then we have

$$m_k(G) = m_k(G - uv) + m_{k-1}(G - u - v),$$
 (5)

$$m_k(G) = m_k(G - u) + \sum_{i=1}^{j} m_{k-1}(G - u - v_i).$$
 (6)

From Lemma 2.1, we know that  $m_k(P_1 \cup G) = m_k(G)$ . And we can also obtain that

**Lemma 2.2** Let G be a simple graph and H be a subgraph(resp. proper subgraph) of G. Then  $G \succeq H(resp. \succ H)$ .

A connected graph with n vertices and n edges is called a unicyclic graph. Obviously, a unicyclic graph has exactly one cycle. A connected graph with n vertices and n+1 edges is called a bicyclic graph. Let  $\mathcal{U}(n)$  be the class of connected unicyclic graphs with n vertices,  $\mathcal{U}(n,d)$  be the class of unicyclic graphs with n vertices and diameter d, where  $1 \leq d \leq n-2$ . Let  $\mathcal{B}(n)$  be the class of bicyclic graphs in  $\mathcal{B}(n)$  with diameter d, where  $1 \leq d \leq n-2$ . Let  $1 \leq n-2$  be the path with  $1 \leq n-2$  with  $1 \leq n-2$  be the path with

When d=1, n=3,  $K_3$  is the unique graph in  $\mathcal{U}(3,1)$ . When d=1,  $n\geq 4$ ,  $\mathcal{U}(n,1)$  contains no graphs. When d=2, n=4,  $\mathcal{U}(4,2)$  has two graphs  $G_{4,2}^1$  and  $G_{4,2}^2$  (see Figure 1). Clearly,  $ME(G_{4,2}^2)>ME(G_{4,2}^1)$ , i.e.,  $G_{4,2}^1$  is the unique graph with minimal matching energy in  $\mathcal{U}(4,2)$ . When  $d=2, n\geq 5$ , the graph obtained by attaching n-3 pendant vertices to a vertex of a triangle is the unique graph in  $\mathcal{U}(n,2)$ . Thus, we just consider the case in which  $3\leq d\leq n-2$ . In section 3 of our 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 matching energy, where the graph  $U_{n,d}$  is shown in Figure 2.



Figure 1: The two graphs in  $\mathcal{U}(4,2)$ .

$$n-d-1$$

 $U_{n,d}$  with  $3 \le d \le n-2$ 

$$n-d-2$$

 $B_{n,d}$  with  $3 \le d \le n-3$ 

Figure 2: The graphs  $U_{n,d}$  and  $B_{n,d}$ .

When d=2,  $n \geq 6$ ,  $\mathcal{B}(n,2)$  has two graphs  $G_{n,2}^1$  and  $G_{n,2}^2$  (see Figure 3). By Lemma 2.1 and simple calculation, we can get  $G_{n,2}^1 \succ G_{n,2}^2$ , hence  $G_{n,2}^2$  is the unique graph in  $\mathcal{B}(n,2)$  with minimal matching energy. Therefore, we only consider the case in which  $3 \leq d \leq n-2$ . In section 4, we will show that  $B_{n,d}$  is the unique graph with minimal matching energy for  $3 \leq d \leq n-3$ , where the graph  $B_{n,d}$  is shown in Figure 2. Furthermore, we also pay our attention to the case d=n-2.

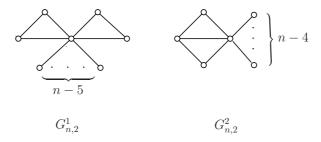


Figure 3: The two graphs in  $\mathcal{B}(n,2)$ .

Let  $\mathcal{T}(n,d)$  be the class of trees with  $n \geq 2$  vertices and diameter d, where  $1 \leq d \leq n-1$ . If  $T \in \mathcal{T}(n,1)$ , then  $T=P_2$ . For  $1 \leq d \leq n-1$ , let  $T_{n,d}$  denote the graph obtained by attaching n-d pendent vertices to an end vertex of  $P_d$ . Specially,  $T_{n,1} = T_{n,2} = S_n$ . Obviously,  $T_{n,2}$  is the unique tree in  $\mathcal{T}(n,2)$  and  $T_{n,n-1} = P_n$  is the unique tree in  $\mathcal{T}(n,n-1)$ .

Let  $G_1, G_2$  be two graphs with n vertices. Now we introduce a quasi-order  $\succeq_1$  defined in [31]: If  $b_i(G_1) \geq b_i(G_2)$  for all  $i \geq 0$ , then we write  $G_1 \succeq_1 G_2$ . If  $G_1 \succeq_1 G_2$  and there exists an  $i_0$  such that  $b_{i_0}(G_1) > b_{i_0}(G_2)$ , then we write  $G_1 \succ_1 G_2$ . The following lemmas are relevant results on this quasi-order.

**Lemma 2.3** ([22, 40]) For  $2 \le i \le \lfloor \frac{n}{2} \rfloor$  and  $n \ge 4$ ,

$$P_n \succ_1 P_i \cup P_{n-i} \succ_1 P_1 \cup P_{n-1}$$
.

**Lemma 2.4** ([19]) For  $3 \le d \le n-2$ ,  $P_n \succeq_1 T_{n,d} \succeq_1 S_n$ .

**Lemma 2.5** ([37]) Let  $T \in \mathcal{T}(n,d)$  and  $T \neq T_{n,d}$ . Then  $T \succ_1 T_{n,d}$ .

**Lemma 2.6 ([29])** If  $d > d_0 \ge 3$ , then  $T_{n,d} \succ_1 T_{n,d_0}$ .

**Lemma 2.7 ([39])** For  $2 \le d_1 \le n_1 - 2$ , we have  $T_{n_1,d_1} \cup T \succeq_1 T_{n_1+n_2-1,d_1+d_2}$ , where  $T = T_{n_2,d_2}$  if  $2 \le d_2 \le n_2 - 2$ , and  $P_2$  if  $P_2 = 2$  and  $P_2 = 1$ .

If G is an acyclic graph, then [22]  $b_{2k}(G) = m_k(G)$  and  $b_{2k+1}(G) = 0$  for all k. Thus, the quasi-order  $\succ_1$  (resp.  $\succeq_1$ ) in Lemmas 2.3–2.7 can be replaced by  $\succ$  (resp.  $\succeq$ ), and the results also work.

By Lemma 2.1 and the definition of the quasi-order  $\succeq$ , it is easy to see that the following lemma holds.

**Lemma 2.8** Let G,  $G' \in \mathcal{U}(n)$  and  $uv(resp.\ u'v')$  be a pendant edge with the pendant vertex  $u(resp.\ u')$  of the graph  $G(resp.\ G')$ . If  $G - u \succeq G' - u'$  and  $G - u - v \succeq G' - u' - v'$ , or  $G - u \succ G' - u'$  and  $G - u - v \succeq G' - u' - v'$ , then  $G \succ G'$ .

The following lemmas will be needed in our paper, which are obtained based on the previous results.

**Lemma 2.9** For 
$$3 \le d \le n - 2$$
,  $B_{n,d} > U_{n,d} > T_{n,d}$ .

*Proof.* Since  $U_{n,d}$  is a proper subgraph of  $B_{n,d}$ , then by Lemma 2.2, we can get  $B_{n,d} \succ U_{n,d}$ . Similarly, we also have  $U_{n,d} \succ T_{n,d}$ .

**Lemma 2.10** For  $3 \le d_0 < d \le n-2$ ,  $U_{n,d} > U_{n,d_0}$ .

Proof. By Lemmas 2.1, 2.2 and 2.6,

$$\begin{array}{lcl} m_k(U_{n,d}) & \geq & m_k(U_{n-1,d-1}) + m_{k-1}(T_{n-2,d-2}) \\ & \geq & m_k(U_{n-1,d-1}) + m_{k-1}(T_{d-1,d-3}) \\ & = & m_k(U_{n,d-1}). \end{array}$$

Furthermore,  $m_2(U_{n,d}) > m_2(U_{n,d-1})$ . It follows that  $U_{n,d} \succ U_{n,d-1}$ . Therefore,  $U_{n,d} \succ U_{n,d-1} \succ \cdots \succ U_{n,d_0}$ .

Similarly, we have

**Lemma 2.11** For  $3 \le d_0 < d \le n-2$ ,  $B_{n,d} > B_{n,d_0}$ .

## 3 Unicyclic graphs with a given diameter

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

**Lemma 3.1** Let  $G \in \mathcal{U}(n, n-2)$  with  $n \geq 8$  and  $G \neq U_{n,n-2}$ . Then  $G \succ U_{n,n-2}$ .

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

If n = 8, then G is isomorphic to one of the following graphs (see Figure 4).

It is easy to get

$$\alpha(U_{8,6}^1) = \mu^8 - 8\mu^6 + 19\mu^4 - 13\mu^2 + 1; \quad \alpha(U_{8,6}^2) = \mu^8 - 8\mu^6 + 18\mu^4 - 11\mu^2 + 1;$$
  
$$\alpha(U_{8,6}^3) = \mu^8 - 8\mu^6 + 18\mu^4 - 12\mu^2 + 1; \quad \alpha(U_{8,6}^4) = \mu^8 - 8\mu^6 + 19\mu^4 - 14\mu^2 + 2;$$

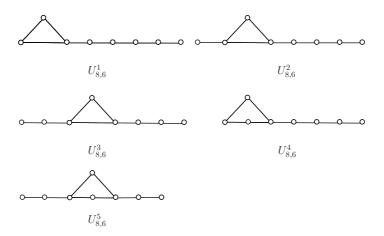


Figure 4: The graphs in  $\mathcal{U}(8,6)$  except for  $U_{8,6}$ .

$$\alpha(U_{8,6}^5) = \mu^8 - 8\mu^6 + 18\mu^4 - 12\mu^2 + 2; \quad \alpha(U_{8,6}) = \mu^8 - 8\mu^6 + 18\mu^4 - 11\mu^2.$$

And then it is obvious that  $U_{8,6}^i \succ U_{8,6}$  for i = 1, 2, 3, 4, 5, i.e.,  $U_{8,6}$  is the unique graph in  $\mathcal{U}(8,6)$  with minimal matching energy.

If n = 9, then G is isomorphic to one of the following graphs (see Figure 5).

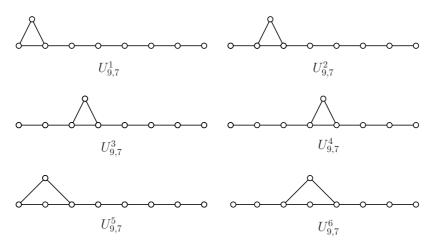


Figure 5: The graphs in  $\mathcal{U}(9,7)$  except for  $U_{9,7}$ .

We can obtain that

$$\begin{split} &\alpha(U_{9,7}^1) = \mu^9 - 9\mu^7 + 26\mu^5 - 26\mu^3 + 6\mu; \quad \alpha(U_{9,7}^2) = \mu^9 - 9\mu^7 + 25\mu^5 - 23\mu^3 + 5\mu; \\ &\alpha(U_{9,7}^3) = \mu^9 - 9\mu^7 + 25\mu^5 - 24\mu^3 + 6\mu; \quad \alpha(U_{9,7}^4) = \mu^9 - 9\mu^7 + 25\mu^5 - 24\mu^3 + 5\mu; \\ &\alpha(U_{9,7}^5) = \mu^9 - 9\mu^7 + 26\mu^5 - 27\mu^3 + 8\mu; \quad \alpha(U_{9,7}^6) = \mu^9 - 9\mu^7 + 25\mu^5 - 24\mu^3 + 6\mu; \end{split}$$

along with

$$\alpha(U_{9,7}) = \mu^9 - 9\mu^7 + 25\mu^5 - 23\mu^3 + 4\mu.$$

It now immediately follows that  $U_{9,7}^i \succ U_{9,7}$  for i = 1, 2, 3, 4, 5, 6, i.e.,  $U_{9,7}$  is the unique graph in  $\mathcal{U}(9,7)$  with minimal matching energy.

Now suppose that the result holds for graphs in  $\mathcal{U}(n-1, n-3)$  and  $\mathcal{U}(n-2, n-4)$ . Let  $G \in \mathcal{U}(n, n-2)$  and  $G \neq U_{n,n-2}$ , where  $n \geq 10$ .

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  $G(\text{resp. }U_{n,n-2})$ . Then the degree of v is 2. So is v'. Hence  $G-u\in\mathcal{U}(n-1,n-3),\ G-u-v\in\mathcal{U}(n-2,n-4)$  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 either  $G - u \neq U_{n-1,n-3}$  or  $G - u - v \neq U_{n-2,n-4}$ . By the induction hypothesis, we have  $G - u \succ U_{n-1,n-3}$  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 2.8,  $G \succ U_{n,n-2}$ .

**Theorem 3.2** Let  $G \in \mathcal{U}(n,d)$  with  $n \geq 8$ ,  $3 \leq d \leq n-2$  and  $G \neq U_{n,d}$ . Then  $ME(G) > ME(U_{n,d})$ .

*Proof.* We prove the result by induction on n-d.

When n-d=2, by Lemma 3.1, we have  $G \succ U_{n,d}$ . Let  $t \geq 3$  and suppose that the result holds for n-d < t. Now suppose that n-d=t. Let u' be the vertex of degree 3 in  $U_{n,d}$  and v' be a vertex on the quadrangle that is adjacent to u'. By Lemma 2.1,

$$m_k(U_{n,d}) = m_k(U_{n,d} - u'v') + m_{k-1}(U_{n,d} - u' - v')$$
  
=  $m_k(T_{n,d}) + m_{k-1}(P_{d-3} \cup S_{n-d+1}).$ 

For  $C_n$ ,  $m_k(C_n) = m_k(P_n) + m_{k-1}(P_{n-2})$ . By Lemma 2.4,  $P_n > T_{n,d}$ . And by Lemmas 2.3 and 2.4,  $P_{n-2} \succeq P_{d-3} \cup P_{n-d+1} \succ P_{d-3} \cup S_{n-d+1}$ . Thus  $C_n \succ U_{n,d}$ . Therefore, we may suppose that the unique cycle of G is  $C_r$  with r < n. Let  $P(G) = v_0 v_1 \dots v_d$  be a diametrical path of G. Then one of  $v_0$  and  $v_d$  must be a pendant vertex.

Case 1 All pendant vertices are on P(G).

Since  $t = n - d \ge 3$ , then  $|V(P(G))| = d + 1 \le n - 2$ . Thus there are at least two adjacency vertices, say u and v, on  $C_r$  which lie outside P(G) such that  $G - uv \in \mathcal{T}(n, d_1)$ , and  $G - u - v \in \mathcal{T}(n - 2, d_2)$ , where  $d_1, d_2 \ge d$ . By Lemmas 2.5 and 2.6,  $G - uv \succeq T_{n,d_1} \succeq T_{n,d}$ ,  $G - u - v \succeq T_{n-2,d_2} \succeq T_{n-2,d}$ . We also have  $T_{n-2,d} \succ P_{d-3} \cup T_{n-d+1,3} \succ P_{d-3} \cup S_{n-d+1}$  by Lemmas 2.2 and 2.4. Hence,  $G - u - v \succ P_{d-3} \cup S_{n-d+1}$ .

Note that  $m_k(G) = m_k(G - uv) + m_{k-1}(G - u - v)$ , so  $m_k(G) \ge m_k(U_{n,d})$  for all k. Moreover, since  $T_{n-2,d} > P_{d-3} \cup S_{n-d+1}$ , there exists some  $k_0$  such that  $m_{k_0-1}(G - u - v) > m_{k_0-1}(P_{d-3} \cup S_{n-d+1})$ , i.e.,  $m_{k_0}(G) > m_{k_0}(U_{n,d})$ . Thus  $G > U_{n,d}$ .

Case 2 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  $U_{n,d}-u'-v'=(n-d-2)P_1\cup T_{d,d-2}$ .

**Subcase 2.1** There is a pendant vertex u outside P(G) such that its neighbor v lies on  $C_r$ .

Since u outside P(G), then  $G - u \in \mathcal{U}(n-1,d)$ . Consequently, by the induction hypothesis,  $G - u \succeq U_{n-1,d}$ .

If v lies outside P(G), then  $G - u - v \supseteq P_{d+1}$ . Thus  $G - u - v \succeq P_{d+1} \succ T_{d,d-2}$ .

Suppose that v lies on P(G), then P(G) and  $C_r$  have common vertices, say  $v_i, \ldots, v_{i+j}$  with  $j \geq 0$ .

If j = 0, i.e.,  $v = v_i$  is the unique common vertex of P(G) and  $C_r$ , then  $G - u - v \supseteq P_i \cup P_{d-i} \cup P_2$ . Since

$$m_k(P_i \cup P_{d-i} \cup P_2) \ge m_k(P_d) \ge m_k(T_{d,d-2})$$

and  $m_2(P_i \cup P_{d-i} \cup P_2) > m_2(T_{d,d-2})$ , then  $P_i \cup P_{d-i} \cup P_2 \succ T_{d,d-2}$ . Therefore,  $G - u - v \succeq P_i \cup P_{d-i} \cup P_2 \succ T_{d,d-2}$ .

If j > 0. For  $v \neq v_i, v_{i+j}, G-u-v \supseteq P_{d+1}$ . So  $G-u-v \succeq P_{d+1} \succ T_{d,d-2}$ . Otherwise, for  $v = v_i$  or  $v_{i+j}$ , say  $v = v_i$ . Then  $G - u - v \supseteq P_i \cup T_1$ , where  $T_1 \in \mathcal{T}(d-i+1, d-i-1)$  is obtained by attaching a pendant vertex to vertex  $v_{i+j}$  of the path  $P = v_{i+1} \cdots v_d$ . For  $k \ge 0$ ,

$$m_k(P_i \cup T_1) \ge m_k(P_i \cup T_{d-i+1,d-i-1}) \ge m_k(T_{d,d-2}).$$

If  $(i,j) \neq (1,2)$ , then  $m_2(P_i \cup T_1) > m_2(T_{d,d-2})$ , hence  $G - u - v \succeq P_i \cup T_1 \succ T_{d,d-2}$ . Otherwise,  $P_i \cup T_1$  is a proper subgraph of G - u - v, then  $G - u - v \succ P_i \cup T_1 \succeq T_{d,d-2}$ . Thus we always have  $G - u - v \succ T_{d,d-2}$ . Therefore,  $G - u - v \succ U_{n,d} - u' - v'$ .

We have proved that  $G - u \succeq U_{n-1,d}$ . Then by Lemma 2.8, we obtain  $G \succ U_{n,d}$ .

**Subcase 2.2** The neighbor of any pendant vertex outside P(G) also lies outside  $C_r$ .

If there is a pendant vertex u such that its neighbor v lies outside P(G), then  $G - u - v \supseteq C_r \cup P_{d+1} \supseteq C_r \cup P_j \cup P_{d-j}$  or  $G - u - v \supseteq G'$ , where  $G' \in \mathcal{U}(s,d)$  with  $d+2 \le s \le n-2$ .

If every pendant vertex outside P(G) is adjacent to 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  $G''\in \mathcal{U}(s',d')$  with  $d'\ge d-j-1$ ,  $s'\ge d'+2$  and  $s'+j\le n-2$ .

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

$$m_k(C_r \cup P_i \cup P_{d-i}) \ge m_k(P_3 \cup P_i \cup P_{d-i}) \ge m_k(T_{d,d-2}).$$

In particular,  $m_1(C_r \cup P_j \cup P_{d-j}) > m_1(T_{d,d-2})$ . Thus,  $G - u - v \succeq C_r \cup P_j \cup P_{d-j} \succ T_{d,d-2}$ .

Next, suppose that  $G - u - v \supseteq G'$ , then  $G - u - v \succeq U_{s,d} \succeq U_{d+2,d} \succ T_{d+2,d}$ .

Finally, suppose that  $G - u - v \supseteq P_j \cup G''$ . For  $G'' \in \mathcal{U}(s', d')$  with  $s' - d' \le n - 2 - j - (d - j - 1) = n - d - 1$ . By the induction hypothesis,  $G'' \succeq U_{s',d'} \succeq U_{d-j+1,d-j-1}$ . Thus

$$G - u - v \succeq P_j \cup G'' \succeq P_j \cup U_{s',d'} \succeq P_j \cup U_{d-j+1,d-j-1}.$$

For  $k \geq 0$ ,

$$m_k(P_j \cup U_{d-j+1,d-j-1}) \ge m_k(P_j \cup T_{d-j+1,d-j-1}) \ge m_k(T_{d,d-2}).$$

Furthermore,  $m_1(P_j \cup U_{d-j+1,d-j-1}) > m_1(T_{d+2,d})$ . It follows that  $G - u - v \succeq P_j \cup U_{d-j+1,d-j-1} \succ T_{d,d-2}$ .

According to the arguments above, we have proved that  $G - u - v > U_{n,d} - u' - v'$ . On the other hand,  $G - u \succeq U_{n-1,d}$ . Thus by Lemma 2.8,  $G > U_{n,d}$ .

Combining Cases 1 and 2, we conclude that  $G \succ U_{n,d}$  also holds for  $G \in \mathcal{U}(n,d)$  with  $3 \leq d \leq n-3$  and  $G \neq U_{n,d}$ , which yields the result.

## 4 Bicyclic graphs with a given diameter

In what follows we state some new definitions and notations. For a graph  $G \in \mathcal{B}(n)$ , it has either two or three distinct cycles. If G has exactly two cycles, suppose that the lengths of them are a and b respectively. If G has three cycles, then any two cycles must have at least one edge in common, and we may choose two cycles of lengths of a and b with t common edges such that  $a - t \geq t$  and  $b - t \geq t$ . Then, in any case, we choose two cycles  $C_a$  and  $C_b$  in G. For convenience, let  $C_a = v_0v_1 \cdots v_{a-1}v_0$  and  $C_b = u_0u_1 \cdots u_{b-1}u_0$ . If  $C_a$  and  $C_b$  have no common edges, then  $C_a$  and  $C_b$  are connected by a unique path P, say from  $v_0$  to  $u_0$ . Let l(G) be the length of P. If  $C_a$  and  $C_b$  have exactly  $t(\geq 1)$  common edges, and thus have exactly t + 1 common vertices, say,  $v_0 = u_0, v_1 = u_1, \ldots, v_t = u_t$ , then  $C_c = u_0u_{b-1} \cdots u_{t+1}u_tv_{t+1}v_{t+2} \cdots v_{a-1}v_0$  is the third cycle of G, where c = b + a - 2t. If we write  $w_0 = u_0, w_1 = u_{b-1}, \ldots, w_{c-1} = v_{a-1}$ , then  $C_c = w_0w_1 \cdots w_{c-1}w_0$ . Denote by d(G) the diameter of G.

Now we turn our attention to the minimal matching energy of graphs in  $\mathcal{B}(n,d)$  with  $3 \le d \le n-2$ . We first deal with the case d=n-3.

**Lemma 4.1** Let  $G \in \mathcal{B}(n, n-3)$  with  $n \geq 7$ , and  $G \neq B_{n,n-3}$ . Then  $G \succ B_{n,n-3}$ .

*Proof.* By induction on n to prove this fact.

For n=7 and n=8, there are only finitely many graphs we need to consider. Then by Lemma 2.1 and direct check, we can get  $G \succ B_{n,n-3}$ .

Suppose that the result holds for all graphs in  $\mathcal{B}(n-1,n-4)$  and  $\mathcal{B}(n-2,n-5)$ , where  $n \geq 9$ . Let  $G \in \mathcal{B}(n,n-3)$  and  $G \neq B_{n,n-3}$ .

Case 1 There is a pendent vertex u in G such that the degree of its neighbor v is 2.

In this case,  $G - u \in \mathcal{B}(n-1, n-4)$  and  $G - u - v \in \mathcal{B}(n-2, n-5)$ . Since  $G \neq B_{n,n-3}$ , then  $G - u \neq B_{n-1,n-4}$  or  $G - u - v \neq B_{n-2,n-5}$ . By the induction hypothesis,  $G - u \succ B_{n-1,n-4}$  and  $G - u - v \succeq B_{n-2,n-5}$ , or  $G - u \succeq B_{n-1,n-4}$  and  $G - u - v \succ B_{n-2,n-5}$ . Hence,  $G \succ B_{n,n-3}$ .

Case 2 The neighbor of any pendent vertex has degree at least 3 or there is no pendent vertex.

Then G is isomorphic to some  $H_j$ , j = 1, 2 (see Figure 6), or G contains one triangle or one quadrangle which has at most one common vertex with the other cycle that is a triangle or a quadrangle.

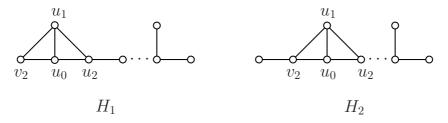


Figure 6: The graphs  $H_i$  for i = 1, 2.

If G is isomorphic to  $H_1$ , then by Lemmas 2.1, 2.5, 2.6 and Theorem 3.2,

$$m_k(G) = m_k(G - u_1v_2) + m_{k-1}(G - u_1 - v_2)$$

$$\geq m_k(U_{n,n-3}) + m_{k-1}(T_{n-2,d-1})$$

$$\geq m_k(U_{n,n-3}) + m_{k-1}(P_{n-6} \cup S_4)$$

$$= m_k(B_{n,n-3}).$$

Moreover,  $m_2(G) > m_2(B_{n,n-3})$ , thus  $G > B_{n,n-3}$ .

If G is isomorphic to  $H_2$ , then by Lemmas 2.1, 2.3 and Theorem 3.2,

$$\begin{array}{lcl} m_k(G) & = & m_k(G-u_1u_0) + m_{k-1}(G-u_1-u_0) \\ & \geq & m_k(U_{n,n-3}) + m_{k-1}(P_2 \cup T_{n-4,n-6}) \\ & \geq & m_k(U_{n,n-3}) + m_{k-1}(P_2 \cup P_{n-5}) + m_{k-2}(P_2 \cup P_{n-7}) \\ & \geq & m_k(U_{n,n-3}) + m_{k-1}(P_3 \cup P_{n-6}) + m_{k-2}(P_{n-6}) \\ & = & m_k(B_{n,n-3}). \end{array}$$

Similarly,  $m_2(G) > m_2(B_{n,n-3})$ , thus  $G > B_{n,n-3}$ .

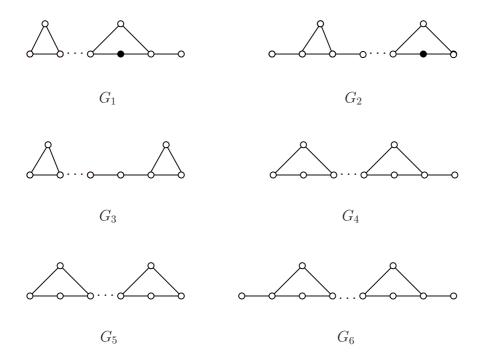


Figure 7: The graphs  $G_i$  for i = 1, 2, 3, 4, 5, 6.

Otherwise, G contains one triangle or one quadrangle which has at most one common vertex with the other cycle that is a triangle or a quadrangle. Choose  $C_a$  and  $C_b$  as above. Let  $b \ge a$ .

If a = 3, then G is isomorphic to  $G_1$ ,  $G_2$  or  $G_3$  in Figure 7, where the black vertices may not occur. Similarly, we can obtain that  $G > B_{n,n-3}$ .

If a=4, then G is isomorphic to  $G_4$ ,  $G_5$  or  $G_6$  in Figure 7. We can show that  $G \succ B_{n,n-3}$  in the same way.

Hence the conclusion follows.

**Lemma 4.2** Let  $G \in \mathcal{B}(n,d)$  with  $n \geq 8$  and  $3 \leq d \leq n-4$ . If G contains no pendent vertices, then  $G \succ B_{n,d+1}$ .

*Proof.* We choose  $C_a$ ,  $C_b$  in G and if there exists the third cycle, then we choose  $C_c$  and t as above. Let  $b \ge a$ . Since  $d \le n - 4$ , we have  $b \ge 5$ .

Case 1  $C_a$  and  $C_b$  have no common edges.

Then  $d = \lfloor \frac{a}{2} \rfloor + \lfloor \frac{b}{2} \rfloor + l(G)$ ,  $d(G - u_1 u_2) = \lfloor \frac{a}{2} \rfloor + l(G) + b - 2 \ge d + 1$ ,  $d(G - u_1 - u_2) = \lfloor \frac{a}{2} \rfloor + l(G) + b - 3 \ge d$ . According to Lemmas 2.1, 2.2,

2.10 and Theorem 3.2,

$$m_k(G) = m_k(G - u_1u_2) + m_{k-1}(G - u_1 - u_2)$$

$$\geq m_k(U_{n,d+1}) + m_{k-1}(U_{n-2,d})$$

$$\geq m_k(U_{n,d+1}) + m_{k-1}(P_{d-2} \cup S_{n-d})$$

$$= m_k(B_{n,d+1}).$$

Further, we have  $m_2(G) > m_2(B_{n,d+1})$ , thus  $G > B_{n,d+1}$ .

Case 2  $C_a$  and  $C_b$  have at least one common edge.

Notice that  $a-t \geq t, b-t \geq t$ , where  $t \geq 1$ . It follows that  $c \geq b+1$ ,  $d = \lfloor \frac{c}{2} \rfloor = \lfloor \frac{(a+b)}{2} \rfloor - t$ ,  $d(G-w_0-w_1) = c-3 \geq d$  and  $d \geq 3$ .

If b > 5 or b = 5 and a is even, then  $d(G - w_0 w_1) = \lfloor \frac{a}{2} \rfloor + b - t - 1 \geq d + 1$ , by Lemmas 2.1, 2.2, 2.9 and Theorem 3.2,

$$m_k(G) = m_k(G - w_0w_1) + m_{k-1}(G - w_0 - w_1)$$

$$\geq m_k(U_{n,d+1}) + m_{k-1}(U_{n-2,d})$$

$$\geq m_k(U_{n,d+1}) + m_{k-1}(T_{n-2,d})$$

$$\geq m_k(U_{n,d+1}) + m_{k-1}(P_{d-2} \cup S_{n-d})$$

$$= m_k(B_{n,d+1})$$

together with  $m_2(G) > m_2(B_{n,d+1})$ , hence  $G > B_{n,d+1}$ .

If b=5 and a is odd, then G is isomorphic to the two graphs in Figure 8, it is easy to verify that  $G > B_{n,d+1}$  and the proof is complete.

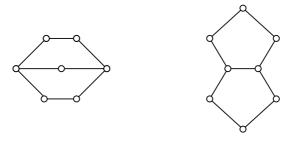


Figure 8: The graphs isomorphic to G when b=5 and a is odd.

**Lemma 4.3** Let  $G \in \mathcal{B}(n,d)$  with  $n \geq 8$  and  $3 \leq d \leq n-4$ . If G contains exactly one pendent vertex u on all diametrical paths of G such that G-u contains no pendent vertices, then  $G \succ B_{n,d+1}$ .

*Proof.* We choose  $C_a$ ,  $C_b$  in G and if there exists the third cycle, then we choose  $C_c$  and t as above. Let  $b \ge a$ . Since  $d \le n - 4$ , we have  $b \ge 5$ . Let v be the neighbor of u.

Case 1  $C_a$  and  $C_b$  have no common edges.

Then  $d = \lfloor \frac{a}{2} \rfloor + \lfloor \frac{b}{2} \rfloor + l(G) + 1$ .

If  $b \geq 7$ , then  $d(G - u_1 u_2) \geq \lfloor \frac{a}{2} \rfloor + l(G) + b - 2 \geq d + 1$ .

If v lies on  $C_a$  and b = 5 or 6, then  $d(G - u_1 u_2) = \lfloor \frac{a}{2} \rfloor + l(G) + b - 1 = d + 1$ .

If v lies on  $C_b$ , a = 5 and b = 6, then  $d(G - v_1v_2) = \lfloor \frac{b}{2} \rfloor + l(G) + a - 1 = d + 1$ .

In these cases, the proof is the same as Case 1 of Lemma 4.2.

Otherwise, v lies on  $C_b$ , a = 3 or 4 and b = 5 or 6.

If l(G) = 0, then G is isomorphic to finitely many graphs. Apply Lemma 2.1 and direct calculation, we can get  $G > B_{n,d+1}$ .

So suppose that  $l(G) \geq 1$ . If a = 3 and b = 5, then  $G - v_0 v_1 \in \mathcal{U}(n, d+1)$ .  $G - v_0 - v_1 = P_1 \cup G_0$ , where  $G_0 \in \mathcal{U}(n-3, d-2)$ . Since  $d(G_0) = d-2$ ,  $n(G_0) = n-3$ , then n-3 = d-2+3, that is, n-d=4, meanwhile, l(G) - 1 = d-2-3 = d-5, i.e., l(G) = d-4. Thus  $G_0 - u_0 u_1 \supseteq P_{d-2} \cup S_3, G_0 - u_0 - u_1 = P_{d-5} \cup P_4$ . Therefore, by Lemmas 2.1, 2.2, 2.3 and Theorem 3.2,

$$m_{k}(G) = m_{k}(G - v_{0}v_{1}) + m_{k-1}(G - v_{0} - v_{1})$$

$$\geq m_{k}(U_{n,d+1}) + m_{k-1}(G_{0} - u_{0}u_{1}) + m_{k-2}(G_{0} - u_{0} - u_{1})$$

$$\geq m_{k}(U_{n,d+1}) + m_{k-1}(P_{d-2} \cup S_{3}) + m_{k-2}(P_{d-2})$$

$$\geq m_{k}(U_{n,d+1}) + m_{k-1}(P_{d-2} \cup S_{n-d})$$

$$= m_{k}(B_{n,d+1}).$$

In particular,  $m_2(G) > m_2(B_{n,d+1})$ , thus  $G > B_{n,d+1}$ .

If a=3 and b=6, by similar arguments, we can obtain that  $G \succ B_{n,d+1}$ . If a=4 and b=5, then n=d+1+3=d+4, i.e., n-d-1=3,  $G-v_0v_1 \in \mathcal{U}(n,d+1)$  and  $G-v_0-v_1=P_2\cup G_0$ , where  $G_0 \in \mathcal{U}(n-4,d-3)$ . Similarly,

$$\begin{array}{lcl} m_k(G) & = & m_k(G-v_0v_1) + m_{k-1}(G-v_0-v_1) \\ & \geq & m_k(U_{n,d+1}) + m_{k-1}(P_2 \cup G_0 - u_0u_1) + m_{k-2}(P_2 \cup G_0 - u_0 - u_1) \\ & \geq & m_k(U_{n,d+1}) + m_{k-1}(P_2 \cup P_{d-2}) + m_{k-2}(P_2 \cup P_{d-6} \cup P_4) \\ & \geq & m_k(U_{n,d+1}) + m_{k-1}(P_3 \cup P_{d-3}) + m_{k-2}(P_{d-2}) \\ & = & m_k(B_{n,d+1}). \end{array}$$

Moreover,  $m_2(G) > m_2(B_{n,d+1})$ , hence  $G > B_{n,d+1}$ .

If a = 4 and b = 6, we can verify that  $G > B_{n,d+1}$  in the same way.

Case 2  $C_a$  and  $C_b$  have at least one common edge.

Then  $d = \lfloor \frac{c}{2} \rfloor + 1 = \lfloor \frac{(a+b)}{2} \rfloor - t + 1$ . Since  $b \geq 5$ ,  $w_0$ ,  $w_1 \neq v$  and  $d(G - w_0 w_1) = \lfloor \frac{a}{2} \rfloor + b - t - 1$ . When  $b \geq 6$ ,  $d(G - w_0 w_1) \geq d + 1$ ,

 $d(G - w_0 w_1) \ge d - 1$ . And then

$$m_k(G) = m_k(G - w_0 w_1) + m_{k-1}(G - w_0 - w_1)$$

$$\geq m_k(U_{n,d+1}) + m_{k-1}(T_{n-2,d-1})$$

$$\geq m_k(U_{n,d+1}) + m_{k-1}(P_{d-2} \cup S_{n-d})$$

$$= m_k(B_{n,d+1})$$

along with  $m_2(G) > m_2(B_{n,d+1})$ , hence  $G > B_{n,d+1}$ . Now, we are left with the cases:

- (i)  $b = 5, t = 2, a = 4, uv \in C_b$ ;
- (ii)  $b = 5, t = 2, a = 4, uv \in C_a$ ;
- (iii) b = 5, t = 2, a = 5.

It can be checked directly that  $G \succ B_{n,d+1}$  in these cases.

Combining Cases 1 and 2, we arrive at the result.

**Theorem 4.4** Let  $G \in \mathcal{B}(n,d)$  with  $n \geq 8$  and  $3 \leq d \leq n-3$ . If there are two vertex-disjoint cycles in G, then  $G \succ B_{n,d}$ .

*Proof.* The proof proceeds by induction on n-d. By Lemma 4.1, the result holds for n-d=3. Let  $h \geq 4$  and assume that the result holds for n-d < h. Suppose that  $G \in \mathcal{B}(n,d)$  with n-d=h.

Case 1 There is no pendent vertex in G.

Then by Lemmas 2.11 and 4.2,  $G \succ B_{n,d+1} \succ B_{n,d}$ .

Case 2 There is a pendent vertex outside some diametrical path  $P(G) = x_0x_1\cdots x_d$ .

Let u, adjacent to v, be a pendent vertex outside P(G) in G. Then  $G - u \in \mathcal{B}(n-1,d)$ . Since (n-1) - d < h, by the induction hypothesis,  $G - u > B_{n-1,d}$ .

By Lemma 2.1,

$$m_k(B_{n,d}) = m_k(B_{n-1,d}) + m_{k-1}(T_{d+1,d-2}) \tag{*}$$

Meanwhile, let H = G - u - v, then

$$m_k(G) = m_k(G-u) + m_{k-1}(G-u-v)$$
  
=  $m_k(G-u) + m_{k-1}(H)$   
 $\geq m_k(B_{n-1,d}) + m_{k-1}(H).$ 

Hence, to complete the proof we shall show that  $m_k(H) \geq m_k(T_{d+1,d-2})$ . Select  $C_a$  and  $C_b$  as above.

**Subcase 2.1** v lies on some cycle, say  $C_a$ . Then  $H \supseteq C_b$ .

First, suppose that P(G) and  $C_b$  have no common vertices. Then  $H \supseteq P_i \cup P_{d-i} \cup C_b$  when v lies on P(G), say  $v = v_i$ . Otherwise,  $H \supseteq P_{d+1} \cup C_b \supseteq P_i \cup P_{d-i} \cup C_b$ . Thus

$$m_k(H) \ge m_k(P_i \cup P_{d-i} \cup C_b) \ge m_k(P_{d-1} \cup S_b) \ge m_k(P_{d-1} \cup P_3)$$
  
  $\ge m_k(P_{d+1}) \ge m_k(T_{d+1,d-2}).$ 

Next, suppose that P(G) and  $C_b$  have common vertices  $x_l, \ldots, x_{l+q}$ , where  $q \geq 0$ .

If v lies outside P(G), then  $H \supseteq G_1$ , where  $G_1 \in \mathcal{U}(s_1, d)$  with  $s_1 \ge d+2$ . Hence,

$$m_k(H) \ge m_k(G_1) \ge m_k(U_{s_1,d}) \ge m_k(T_{s_1,d}) \ge m_k(P_{d+1}) \ge m_k(T_{d+1,d-2}).$$

So suppose that v lies on P(G). Then P(G) and  $C_a$  have common vertices, say  $x_i, \ldots, x_{i+p}$ , where  $p \geq 0$ .

When p = 0, then  $i \ge 1$ , thus  $H \supseteq P_2 \cup P_i \cup G_2$ , where  $G_2 \in \mathcal{U}(s_2, d_2)$ ,  $d_2 \ge d - i - 1 \ge 1$  and  $s_2 \ge d_2 + 2$ . If  $d_2 = 1, i = d - 2$ , then  $G_2 = C_3$ . Therefore,

$$m_k(H) \ge m_k(P_2 \cup P_{d-2} \cup C_3) \ge m_k(P_{d-1} \cup P_3) \ge m_k(P_{d+1}) \ge m_k(T_{d+1,d-2}).$$

If  $d_2 = 2$ , then  $s_2 > 4$ , i > d - 3. Consequently,

$$m_k(H) \ge m_k(P_2 \cup P_i \cup G_2) \ge m_k(P_2 \cup P_i \cup S_{s_2}) \ge m_k(P_2 \cup P_i \cup T_{4,2})$$
  
  $\ge m_k(T_{i+4,i+2}) \ge m_k(T_{d+1,d-1}) \ge m_k(T_{d+1,d-2}).$ 

If  $d_2 \geq 3$ , then  $s_2 \geq 5$ . Thus

$$m_k(H) \geq m_k(P_2 \cup P_i \cup G_2) \geq m_k(P_2 \cup P_i \cup U_{s_2,d_2}) \geq m_k(P_2 \cup P_i \cup T_{s_2,d_2})$$
  
$$\geq m_k(T_{s_2+i,d_2+i}) \geq m_k(T_{d_2+i+2,d_2+i}) \geq m_k(T_{d+1,d-1}) \geq m_k(T_{d+1,d-2}).$$

When p = 1. If  $v = v_i$ , then  $i \ge 1$  and  $H \supseteq P_i \cup G_3$ , where  $G_3 \in \mathcal{U}(s_3, d_3), d_3 \ge d - i \ge 3, s_3 \ge d_3 + 2$ . Accordingly,

$$m_k(H) \ge m_k(P_i \cup G_3) \ge m_k(P_i \cup U_{s_3,d_3}) \ge m_k(P_i \cup T_{s_3,d_3}) \ge m_k(T_{s_3+i-1,d_3+i-1})$$
  
  $\ge m_k(T_{d_2+i+2,d_2+i}) \ge m_k(T_{d+1,d-1}) \ge m_k(T_{d+1,d-2}).$ 

If  $v = v_{i+1}$ , then  $H \supseteq P_{i+2} \cup G_4$ , where  $G_4 \in \mathcal{U}(s_4, d_4), d_4 \ge d - (i+1) - 1 = d - i - 2 \ge 1, s_4 \ge d_4 + 2$ .

If  $d_4 = 1$ , then i = d - 3,  $G_4 = C_3$ , we have

$$m_k(H) > m_k(P_{d-1} \cup C_3) > m_k(P_{d-1} \cup P_3) > m_k(P_{d+1}) > m_k(T_{d+1 d-2}).$$

If  $d_4 = 2$ , then  $s_4 \ge 4$ ,  $i \ge d - 4$ . Consequently,

$$m_k(H) \ge m_k(P_{i+2} \cup G_4) \ge m_k(P_{i+2} \cup S_{s_4}) \ge m_k(P_{i+2} \cup T_{4,2})$$
  
  $\ge m_k(T_{i+5,i+3}) \ge m_k(T_{d+1,d-1}) \ge m_k(T_{d+1,d-2}).$ 

If  $d_4 \geq 3$ . Then

$$m_k(H) \ge m_k(P_{i+2} \cup G_4) \ge m_k(P_{i+2} \cup U_{s_4,d_4}) \ge m_k(P_{i+2} \cup T_{s_4,d_4})$$
  
  $\ge m_k(T_{s_4+i+1,d_4+i+1}) \ge m_k(T_{d+1,d-1}) \ge m_k(T_{d+1,d-2}).$ 

Now suppose that  $p \geq 2$ . If  $v \neq x_i$ ,  $x_{i+p}$ , then  $H \supseteq G_5$ , where  $G_5 \in \mathcal{U}(s_5, d_5), d_5 \geq d, s_5 \geq d_5 + 2$ . Hence

$$m_k(H) \ge m_k(G_5) \ge m_k(U_{s_5,d_5}) \ge m_k(T_{s_5,d_5}) \ge m_k(T_{d+1,d-2}).$$

If  $v = x_i$ , then  $H \supseteq P_i \cup G_6$ , where  $G_6 \in \mathcal{U}(s_6, d_6), d_6 \ge d - i - 1 \ge 3, s_6 \ge d_6 + 3$ . Therefore,

$$m_k(H) \ge m_k(P_i \cup G_6) \ge m_k(P_i \cup U_{s_6,d_6}) \ge m_k(P_i \cup T_{s_6,d_6})$$
  
  $\ge m_k(T_{s_6+i-1,d_6+i-1}) \ge m_k(T_{d+1,d-2}).$ 

If  $v = x_{i+p}$ , then  $H \supseteq T_1 \cup G_7$  or  $P_{i+p+1} \cup G_7$ , where  $G_7 \in \mathcal{U}(s_7, d_7), d_7 \ge d-i-p-1 \ge 1, s_7 \ge d_7 + 2, T_1 \in \mathcal{T}(i+p+1, d_{T_1}), d_{T_1} \ge i+p-1$ . If  $d_7 = 1$ , then  $i+p=d-2, G_7 = C_3$ , thus

$$m_k(H) \ge m_k(T_{d-1,d-3} \cup C_3) \ge m_k(T_{d-1,d-3} \cup P_3) \ge m_k(T_{d+1,d-2})$$

or

$$m_k(H) \ge m_k(P_{i+p+1} \cup G_7) \ge m_k(P_{i+p+1} \cup C_3) \ge m_k(P_{i+p+1} \cup P_3)$$
  
  $\ge m_k(P_{i+p+3}) = m_k(P_{d+1}) \ge m_k(T_{d+1,d-2}).$ 

If  $d_7 = 2$ , then  $i + p \ge d - 3$ ,  $s_7 \ge 4$ , accordingly,

$$m_k(H) \ge m_k(T_{i+p+1,i+p-1} \cup S_{s_7}) \ge m_k(T_{i+p+1,i+p-1} \cup T_{4,2})$$
  
  $\ge m_k(T_{i+p+4,i+p+1}) \ge m_k(T_{d+1,d-2})$ 

or

$$m_k(H) \ge m_k(P_{i+p+1} \cup S_{s_7}) \ge m_k(P_{i+p+1} \cup T_{4,2}) \ge m_k(T_{i+p+4,i+p+2}) \ge m_k(T_{d+1,d-2}).$$

If  $d_7 \geq 3$ , then

$$m_k(H) \ge m_k(T_{i+p+1,i+p-1} \cup U_{s_7,d_7}) \ge m_k(T_{i+p+1,i+p-1} \cup T_{s_7,d_7})$$
  
  $\ge m_k(T_{i+p+s_7,i+p+d_7-1}) \ge m_k(T_{d+1,d-2})$ 

or

$$m_k(H) \ge m_k(P_{i+p+1} \cup U_{s_7,d_7}) \ge m_k(P_{i+p+1} \cup T_{s_7,d_7}) \ge m_k(T_{i+p+s_7,i+p+d_7}) \ge m_k(T_{d+1,d-2}).$$

**Subcase 2.2** v lies outside any cycle. Then  $H \supseteq C_a \cup C_b$ .

First, suppose that v lies on P(G) and take  $v = x_i$ . If P(G) has no common vertices with any cycle, then  $H \supseteq C_a \cup C_b \cup P_i \cup P_{d-i}$ . Thus

$$m_k(H) \ge m_k(C_a \cup C_b \cup P_i \cup P_{d-i}) \ge m_k(P_3 \cup P_{d-1}) \ge m_k(P_{d+1}) \ge m_k(T_{d+1,d-2}).$$

If P(G) has no common vertices with exactly one cycle, say  $C_a$ . Then  $H \supseteq C_a \cup P_i \cup G_1$ , where  $G_1 \in \mathcal{U}(s_1, d_1), d_1 \ge d - i - 1, s_1 \ge d_1 + 2$ . If  $d_1 = 1$ , then  $i = d - 2, G_1 = C_3$ , hence

$$m_k(H) \geq m_k(C_a \cup P_i \cup C_3) \geq m_k(P_2 \cup P_i \cup P_3) \geq m_k(P_{i+3}) = m_k(P_{d+1}) \geq m_k(T_{d+1,d-2}).$$

If  $d_1 = 2$ , then  $i \ge d - 3$ ,  $s_1 \ge 4$ . Consequently,

$$m_k(H) \ge m_k(C_a \cup P_i \cup G_1) \ge m_k(P_2 \cup P_i \cup T_{s_1,2}) \ge m_k(T_{i+s_1,i+2}) \ge m_k(T_{d+1,d-2}).$$

If  $d_1 \geq 3$ , then

$$m_k(H) \geq m_k(C_a \cup P_i \cup G_1) \geq m_k(P_2 \cup P_i \cup U_{s_1,d_1}) \geq m_k(P_2 \cup P_i \cup T_{s_1,d_1})$$
  
$$\geq m_k(P_{i+1} \cup T_{s_1,d_1}) \geq m_k(T_{s_1+i,d_1+i}) \geq m_k(T_{d+1,d-2}).$$

If P(G) has common vertices with both cycles, then  $H \supseteq P_i \cup G_2$  or  $G_3 \cup G_4$ , where  $G_2 \in \mathcal{U}(s_2, d_2), \ G_3 \in \mathcal{U}(s_3, d_3), \ G_4 \in \mathcal{U}(s_4, d_4)$ . Meanwhile,  $d_2 \ge d - i - 1 \ge 3, \ n - 2 - i \ge s_2 \ge d_2 + 3, \ d_3 \ge i - 1 \ge 1, \ s_3 \ge d_3 + 2, \ d_4 \ge d - i - 1 \ge 1, \ s_4 \ge d_4 + 2$ .

Suppose that  $H \supseteq P_i \cup G_2$ . Since  $s_2 - d_2 \le n - 2 - i - (d - i - 1) = n - d - 1 < h$ , thus by the induction hypothesis,  $G_2 \succ B_{s_2,d_2}$ . Then

$$m_k(H) \ge m_k(P_i \cup G_2) \ge m_k(P_i \cup B_{s_2,d_2}) \ge m_k(P_i \cup T_{s_2,d_2})$$
  
  $\ge m_k(T_{s_2+i-1,d_2+i-1}) \ge m_k(T_{d+1,d-2}).$ 

Suppose that  $H \supseteq G_3 \cup G_4$ . If  $d_3 = d_4 = 1$ , then n = 8, d = 4,  $G_3 = G_4 = G_3$ . In this case, it is easy to obtain that  $G \succ B_{8,4}$ .

If  $d_3 = 2$ ,  $d_4 = 1$ , then d = 5,  $s_3 \ge 4$ ,  $G_4 = C_3$ . We can have

$$m_k(H) \ge m_k(G_3 \cup G_4) \ge m_k(S_{s_3} \cup G_3) \ge m_k(T_{4,2} \cup P_3) \ge m_k(T_{6,4}) \ge m_k(T_{d+1,d-2}).$$

If  $d_3 \geq 3$ ,  $d_4 = 1$ , then  $d_3 \geq d - 3$ . Accordingly,

$$m_k(H) \ge m_k(G_3 \cup G_4) \ge m_k(U_{s_3,d_3} \cup C_3) \ge m_k(T_{s_3,d_3} \cup P_3)$$
  
  $\ge m_k(T_{s_3+2,d_3+2}) \ge m_k(T_{d+1,d-2}).$ 

If  $d_3 = 2$ ,  $d_4 = 2$ , then d = 6,  $s_3 \ge 4$ ,  $s_4 \ge 4$ . Hence

$$m_k(H) \ge m_k(G_3 \cup G_4) \ge m_k(S_{s_3} \cup S_{s_4}) \ge m_k(T_{4,2} \cup T_{4,2}) \ge m_k(T_{7,4}) = m_k(T_{d+1,d-2}).$$

If  $d_3 \ge 3$ ,  $d_4 = 2$ , then  $d_3 \ge d - 4$ ,  $s_4 \ge 4$ . Thus

$$m_k(H) \ge m_k(G_3 \cup G_4) \ge m_k(U_{s_3,d_3} \cup S_{s_4}) \ge m_k(T_{s_3,d_3} \cup T_{s_4,2})$$
  
  $\ge m_k(T_{s_3+s_4-1,d_3+2}) \ge m_k(T_{d+1,d-2}).$ 

If  $d_3 \geq 3$ ,  $d_4 \geq 3$ , then  $d_3 + d_4 \geq d - 2$ . Therefore,

$$m_k(H) \ge m_k(G_3 \cup G_4) \ge m_k(U_{s_3,d_3} \cup U_{s_4,d_4}) \ge m_k(T_{s_3,d_3} \cup T_{s_4,d_4})$$
  
  $\ge m_k(T_{s_3+s_4-1,d_3+d_4}) \ge m_k(T_{d+1,d-2}).$ 

Next, suppose that v lies outside P(G). Then  $H \supseteq C_a \cup C_b \cup P(G)$ ,  $C_a \cup G_5$  or  $G_6$ , where  $G_5 \in \mathcal{U}(s_5, d)$  with  $s_5 \ge d + 2$  and  $G_6 \in \mathcal{B}(s_6, d)$  with  $d+3 \le s_6 \le n-2$ . It is easy to show as above that  $m_k(H) \ge m_k(T_{d+1,d-2})$ .

Case 3 Any diametrical path of G contains all pendent vertices.

Let  $P(G) = x_0x_1 \cdots x_d$  be any diametrical path of G. Suppose that  $y_0y_1 \cdots y_p$  is a path whose internal vertices  $y_1, y_2, \ldots, y_{p-1}$  all have degree two and  $y_p$  is a pendent vertex. Then we call it a pendent path, denoted by  $(y_0, y_p)$ .

**Subcase 3.1** There are exactly two pendent vertices in G, namely,  $x_0$  and  $x_d$ .

Suppose that  $deg_G(x_i)$ ,  $deg_G(x_l) \geq 3$  such that  $(x_i, x_0)$  and  $(x_l, x_d)$  are distinct pendent paths. Let s = l - i.

If s = 0, i.e.,  $x_i = x_l$ . Then  $i \ge 3, l \le d - 3$ . Since

$$\begin{array}{lll} m_k(G) & = & m_k(G-x_{i-3}x_{i-2}) + m_{k-1}(G-x_{i-3}-x_{i-2}) \\ & = & m_k(G-x_{i-3}x_{i-2}-x_{l+1}x_{l+2}) + m_{k-1}(G-x_{i-3}x_{i-2}-x_{l+1}-x_{l+2}) \\ & & + m_{k-1}(G-x_{i-3}-x_{i-2}-x_{l+2}x_{l+3}) + m_{k-2}(G-x_{i-3}-x_{i-2}-x_{l+2}-x_{l+3}) \\ & = & m_k(G_1 \cup P_{i-2} \cup P_{d-i-1}) + m_{k-1}(G_3 \cup P_{i-2} \cup P_{d-i-2}) \\ & & + m_{k-1}(G_2 \cup P_{i-3} \cup P_{d-i-2}) + m_{k-2}(G_4 \cup P_{i-3} \cup P_{d-i-3}) \end{array}$$

and

$$m_k(B_{n,d}) = m_k(B_{n-d+3,3} \cup P_{d-3}) + m_{k-1}(S_{n-d+2} \cup P_{d-4})$$

$$= m_k(B_{n-d+3,3} \cup P_{i-2} \cup P_{d-i-1}) + m_{k-1}(B_{n-d+3,3} \cup P_{i-3} \cup P_{d-i-2})$$

$$+ m_{k-1}(S_{n-d+2} \cup P_{i-2} \cup P_{d-i-2}) + m_{k-2}(S_{n-d+2} \cup P_{i-3} \cup P_{d-i-3}),$$

it suffices to prove that  $G_1, G_2 \succ B_{n-d+3,3}$  and  $G_3, G_4 \succ S_{n-d+2}$ , where  $G_1 = G - (x_{i-3}, x_0) - (x_{l+2}, x_d) \in \mathcal{B}(n-d+3, d_1), G_2 = G - (x_{i-2}, x_0) - (x_{l+3}, x_d) \in \mathcal{B}(n-d+3, d_2), G_3 = G - (x_{i-3}, x_0) - (x_{l+1}, x_d), G_4 = G - (x_{i-2}, x_0) - (x_{l+2}, x_d), d_1 \ge 4, d_2 \ge 4$ . Since  $n-d+3-d_1 \le n-d-1 < h$ ,  $n-d+3-d_2 \le n-d-1 < h$ . Then by the induction hypothesis,  $G_1 \succ B_{n-d+3,d_1} \succ B_{n-d+3,3}, G_2 \succ B_{n-d+3,d_2} \succ B_{n-d+3,3}$ . In addition, both  $G_3$  and  $G_4$  are bicyclic graphs with n-d+2 vertices, consequently, we have  $G_3, G_4 \succ S_{n-d+2}$ .

If s = 1 or s = 2, then by similar arguments as above, we have the desired result.

If  $s \geq 3$ , it is easy to obtain that  $i \geq 2$  and  $l \leq d-2$ . Then

$$\begin{array}{lll} m_k(G) & = & m_k(G-x_{i-2}x_{i-1}) + m_{k-1}(G-x_{i-2}-x_{i-1}) \\ & = & m_k(G-x_{i-2}x_{i-1}-x_{l+1}x_{l+2}) + m_{k-1}(G-x_{i-2}x_{i-1}-x_{l+1}-x_{l+2}) \\ & & + m_{k-1}(G-x_{i-2}-x_{i-1}-x_{l+1}x_{l+2}) + m_{k-2}(G-x_{i-2}-x_{i-1}-x_{l+1}-x_{l+2}) \\ & = & m_k(G_5 \cup P_{i-1} \cup P_{d-l-1}) + m_{k-1}(G_7 \cup P_{i-1} \cup P_{d-l-2}) \\ & & + m_{k-1}(G_6 \cup P_{i-2} \cup P_{d-l-1}) + m_{k-2}(G_8 \cup P_{i-2} \cup P_{d-l-2}), \end{array}$$

$$\begin{array}{lll} m_k(B_{n,d}) & = & m_k(B_{n-d+l+1,l+1} \cup P_{d-l-1}) + m_{k-1}(B_{n-d+l,l} \cup P_{d-l-2}) \\ & = & m_k(B_{n-d+s+2,s+2} \cup P_{i-1} \cup P_{d-l-1}) + m_{k-1}(B_{n-d+s+1,s+1} \cup P_{i-2} \cup P_{d-l-1}) \\ & & + & m_{k-1}(B_{n-d+s+1,s+1} \cup P_{i-1} \cup P_{d-l-2}) + m_{k-2}(B_{n-d+s,s} \cup P_{i-2} \cup P_{d-l-2}). \end{array}$$

Hence it suffices to show that  $G_5 \succ B_{n-d+s+2,s+2}$ ,  $G_6, G_7 \succ B_{n-d+s+1,s+1}$ ,  $G_8 \succ B_{n-d+s,s}$ .

Let  $d_j = d(G_j)$ , and  $n_j = |V(G_j)|$ , where j = 5, 6, 7, 8. Then  $d_j \geq 4$ . If  $n_j - d_j < h$  holds for all  $j \in \{5, 6, 7, 8\}$ , then by the induction hypothesis and previous Lemmas, we have the desired results. Otherwise, there exists at least a  $j \in \{5, 6, 7, 8\}$  such that  $n_j - d_j = h$ . When j = 5,  $G_5 \in \mathcal{B}(n-d+s+2,s+2)$ . If there exists some diametrical path  $P(G_5)$  such that  $x_{i-1}$  or  $x_{l+1}$  lies outside  $P(G_5)$ , the proof is similar with Case 2, thus  $G_5 \succ B_{n-d+s+2,s+2}$ . Otherwise,  $G_5 - x_{i-1} \in \mathcal{B}(n-d+s+1,s+1)$ , then by Lemma 4.3,  $G_5 \succ B_{n-d+s+1,s+2}$ . We also have  $G_5 - x_{i-1} - x_i \succeq U_{n-d+s,s} \succ T_{n-d+s,s} \succ T_{s+3,s}$ . Therefore,  $G_5 \succ B_{n-d+s+2,s+2}$ .

When j = 7,  $G_7 \in \mathcal{B}(n-d+s+1,s+1)$ . If  $x_{i-1}$  lies on all diametrical paths of  $G_7$ , then by Lemma 4.3,  $G_7 \succ B_{n-d+s+1,s+2} \succ B_{n-d+s+1,s+1}$ . Otherwise, in the same way as in Case 2, we can also obtain  $G_7 \succ B_{n-d+s+1,s+1}$ .

Similarly, when j = 6, we can have  $G_6 > B_{n-d+s+1,s+1}$ .

When j = 8,  $G_8 \in \mathcal{B}(n-d+s,s)$ . Since  $G_8$  contains no pendent vertices, then by Lemmas 2.11 and 4.2,  $G_8 \succ B_{n-d+s,s+1} \succ B_{n-d+s,s}$ .

**Subcase 3.2** There is only one pendent vertex in G, say  $x_0$ .

Since there are two vertex-disjoint cycles in G,  $deg_G(x_d) = 2$ . Suppose that  $x_l$  is the vertex such that  $deg_G(x_l) \geq 3$  and  $deg_G(x_i) = 2$  for  $l+1 \leq i \leq d$ . It is easy to check that  $l \leq d-2$ . Then  $G - x_{d-1}x_d \in \mathcal{U}(n, d_9)$ , where  $d_9 \geq d$ , and  $G - x_{d-1} - x_d \in \mathcal{U}(n-2, d_{10})$ , where  $d_{10} \geq d-1$ . Hence,

$$m_k(G) = m_k(G - x_{d-1}x_d) + m_{k-1}(G - x_{d-1} - x_d)$$

$$\geq m_k(U_{n,d_9}) + m_{k-1}(U_{n-2,d_{10}})$$

$$\geq m_k(U_{n,d}) + m_{k-1}(U_{n-2,d-1})$$

$$\geq m_k(U_{n,d}) + m_{k-1}(T_{n-2,d-1})$$

$$\geq m_k(U_{n,d}) + m_{k-1}(P_{d-3} \cup S_{n-d+1})$$

$$= m_k(B_{n,d}).$$

In particular,  $m_2(G) > m_2(B_{n,d})$ . Thus,  $G \succ B_{n,d}$ . Therefore, we complete the proof.

**Theorem 4.5** Let  $G \in \mathcal{B}(n,d)$  with  $n \geq 8$ ,  $3 \leq d \leq n-3$  and  $G \neq B_{n,d}$ . If there is no vertex-disjoint cycles in G, then  $G \succ B_{n,d}$ .

*Proof.* We will prove this theorem by induction on n-d.

By Lemma 4.1, the result holds for n-d=3. Let  $h \geq 4$  and suppose that the result holds for n-d < h. Now assume that n-d=h, let  $G \in \mathcal{B}(n,d)$  and  $G \neq B_{n,d}$ .

Case 1 If G contains no pendent vertices.

Then by Lemmas 2.11 and 4.2,  $G \succ B_{n,d+1} \succ B_{n,d}$ .

Case 2 If there exists a pendent vertex outside some diametrical path  $P(G) = x_0 x_1 \dots x_d$ .

Let u be a pendent vertex outside P(G) and v be its unique neighbor. Then  $G - u \in \mathcal{B}(n-1,d)$ . If  $G - u = B_{n-1,d}$ , then it can be checked that  $G - u - v \succ T_{d+1,d-2}$ . And thus from (\*), we can obtain that  $G \succ B_{n,d}$ . Otherwise, by the induction hypothesis, we have  $G - u \succ B_{n-1,d}$ . Let H = G - u - v, in order to prove the result, we only need to show that  $m_k(H) \ge m_k(T_{d+1,d-2})$ . We choose  $C_a$ ,  $C_b$  as above in G, and if there exists the third cycle, denote it by  $C_c$ .

**Subcase 2.1** When v lies on some cycle, say  $C_a$ .

First, suppose that  $v = u_0$  or  $u_t$ , then H contains no cycles. If v lies outside P(G), then  $H \supseteq P(G)$ . Thus  $m_k(H) \ge m_k(P(G)) = m_k(P_{d+1}) \ge m_k(T_{d+1,d-2})$ . If v lies on P(G), say  $v = x_i$ .

(1) If  $C_a$  and  $C_b$  have exactly one common vertex, then  $H \supseteq P_2 \cup P_2 \cup P_i \cup P_{d-i}$ ,  $P_2 \cup P_i \cup P_{d-i+1}$ ,  $P_2 \cup P_{i+1} \cup P_{d-i}$ ,  $P_{i+1} \cup P_{d-i+1}$ ,  $P_2 \cup P_i \cup T_1$ ,  $P_2 \cup P_{d-i} \cup T_2$ ,  $P_{i+1} \cup T_1$ ,  $P_{d-i+1} \cup T_2$  or  $T_1 \cup T_2$ , where  $T_1 \in \mathcal{T}(d-i+1, d-i-1)$  and  $T_2 \in \mathcal{T}(i+1, i-1)$ .

If  $H \supseteq P_2 \cup P_2 \cup P_i \cup P_{d-i}$ ,  $P_2 \cup P_i \cup P_{d-i+1}$ ,  $P_2 \cup P_{i+1} \cup P_{d-i}$  or  $P_{i+1} \cup P_{d-i+1}$ , then  $m_k(H) \ge m_k(P_{d+1}) \ge m_k(T_{d+1,d-2})$ ;

If  $H \supseteq P_2 \cup P_i \cup T_1$ , then  $m_k(H) \ge m_k(P_{i+1} \cup T_1) \ge m_k(P_{i+1} \cup T_1)$  $T_{d-i+1,d-i-1}) \ge m_k(T_{d+1,d-1}) \ge m_k(T_{d+1,d-2})$ ; Similarly, if  $H \supseteq P_2 \cup P_{d-i} \cup T_2$ , we also have  $m_k(H) \ge m_k(T_{d+1,d-2})$ ;

If  $H \supseteq T_1 \cup T_2$ , then  $m_k(H) \ge m_k(T_1 \cup T_2) \ge m_k(T_{d-i+1,d-i-1} \cup T_{i+1,i-1}) \ge m_k(T_{d+1,d-2})$ ;

If  $H \supseteq P_{i+1} \cup T_1$  or  $H \supseteq P_{d-i+1} \cup T_2$ , then  $m_k(H) \ge m_k(T_1 \cup T_2) \ge m_k(T_{d+1,d-2})$ .

(2) If  $C_a$  and  $C_b$  have at least two common vertices, then  $H \supseteq P_3 \cup P_i \cup P_{d-i}$ ,  $P_i \cup P_{d-i+2}$ , P(G),  $P_i \cup T_3$  or  $P_i \cup T_4$ , where  $T_3 \in \mathcal{T}(d-i+2, d-i-1)$  and  $T_4 \in \mathcal{T}(d-i+2, d-i)$ .

If  $H \supseteq P_3 \cup P_i \cup P_{d-i}$ ,  $P_i \cup P_{d-i+2}$  or P(G), then  $m_k(H) \ge m_k(P_{d+1}) \ge m_k(T_{d+1,d-2})$ ;

If  $H \supseteq P_i \cup T_3$ , then  $m_k(H) \ge m_k(P_i \cup T_3) \ge m_k(P_i \cup T_{d-i+2,d-i-1}) \ge m_k(T_{d+1,d-2})$ ;

If  $H \supseteq P_i \cup T_4$ , then  $m_k(H) \ge m_k(P_i \cup T_4) \ge m_k(P_i \cup T_{d-i+2,d-i}) \ge m_k(T_{d+1,d-1}) \ge m_k(T_{d+1,d-2})$ .

Next, suppose that  $v \neq u_0$  and  $v \neq u_t$ . If v lies outside P(G), then  $H \supseteq P(G)$ , similarly, we have  $m_k(H) \ge m_k(T_{d+1,d-2})$ . So suppose that v lies on P(G). Then P(G) and  $C_a$  have common vertices, say  $x_i, \ldots, x_{i+p}$ , where  $p \ge 0$ .

(1) If p=0, then  $i\geq 1$  and  $H\supseteq P_i\cup P_{d-i}\cup C_s$ , where s=b or c. It

follows that

$$m_k(H) \ge m_k(P_i \cup P_{d-i} \cup C_s) \ge m_k(P_i \cup P_{d-i} \cup S_s) \ge m_k(P_i \cup P_{d-i} \cup P_3)$$
  
  $\ge m_k(P_{d+1}) \ge m_k(T_{d+1,d-2}).$ 

(2) If  $p \geq 1$ . When  $v \neq x_i$  and  $v \neq x_{i+p}$ , then  $H \supseteq G_1$ , where  $G_1 \in \mathcal{U}(s_1, d_1)$ ,  $d_1 \geq d$  and  $s_1 \geq d_1 + 2$ . Thus

$$m_k(H) \ge m_k(G_1) \ge m_k(U_{s_1,d_1}) \ge m_k(T_{s_1,d_1}) \ge m_k(T_{s_1,d}) \ge m_k(T_{d+1,d-2}).$$

When  $v = x_i$  or  $x_{i+p}$ , say  $v = x_i (i \ge 1)$ , then  $H \supseteq P_i \cup G_2$ , where  $G_2 \in \mathcal{U}(s_2, d_2)$ ,  $d_2 \ge d - i - 1 \ge 2$   $(d - i - 1 \ge 1$ , for d - i - 1 = 1, clearly  $m_k(H) \ge m_k(T_{i+3,i})$  and  $s_2 \ge d - i + 2$ ; or  $H \supseteq P_i \cup G_3$ , where  $G_3 \in \mathcal{U}(s_3, d_3)$ ,  $d_3 \ge d - i \ge 2$  and  $s_3 \ge d_3 + 2$ ; or  $H \supseteq P_i \cup G'$ , where G' is the graph obtained by attaching a path  $P_{d-i-2}$  to a vertex of  $C_b = C_3$ .

Suppose that  $H \supseteq P_i \cup G_2$ . If  $d_2 = 2$ , then i = d - 3 and  $s_2 \ge 5$ . Hence,

$$m_k(H) \ge m_k(P_i \cup G_2) \ge m_k(P_i \cup S_{s_2}) \ge m_k(P_i \cup T_{5,2}) \ge m_k(T_{i+4,i+1}) = m_k(T_{d+1,d-2}).$$

If  $d_2 > 3$ , then

$$m_k(H) \ge m_k(P_i \cup G_2) \ge m_k(P_i \cup U_{s_2,d_2}) \ge m_k(P_i \cup T_{s_2,d_2})$$
  
  $\ge m_k(T_{i+s_2-1,i+d_2-1}) \ge m_k(T_{d+1,d-1}) \ge m_k(T_{d+1,d-2}).$ 

Suppose that  $H \supseteq P_i \cup G_3$ . If  $d_3 = 2$ , then i = d - 2 and  $s_3 \ge 4$ . Thus

$$m_k(H) \ge m_k(P_i \cup G_3) \ge m_k(P_i \cup S_{s_3}) \ge m_k(P_i \cup T_{4,2})$$
  
  $\ge m_k(T_{d+1,d-1}) \ge m_k(T_{d+1,d-2}).$ 

If  $d_3 \geq 3$ , then

$$m_k(H) \ge m_k(P_i \cup G_3) \ge m_k(P_i \cup U_{s_3,d_3}) \ge m_k(P_i \cup T_{s_3,d_3})$$
  
  $\ge m_k(T_{i+s_3-1,i+d_3-1}) \ge m_k(T_{d+1,d-1}) \ge m_k(T_{d+1,d-2}).$ 

Suppose that  $H \supseteq P_i \cup G'$ . If d-i-2=0, then i=d-2 and  $H \supseteq P_i \cup C_3$ . Therefore,

$$m_k(H) \ge m_k(P_i \cup G') \ge m_k(P_i \cup T_{4,2}) \ge m_k(T_{i+3,i+1}) = m_k(T_{d+1,d-1}) \ge m_k(T_{d+1,d-2}).$$

If  $d-i-2 \ge 1$ , choose an edge  $u_0u_1$  of G' in  $C_3$  such that both  $u_0$  and  $u_1$  have degree 2. Then

$$\begin{array}{lcl} m_k(H) & \geq & m_k(P_i \cup G') \\ & = & m_k(P_i \cup G' - u_0 u_1) + m_{k-1}(P_i \cup G' - u_0 - u_1) \\ & = & m_k(P_i \cup T_{d-i+1,d-i-1}) + m_{k-1}(P_i \cup P_{d-i-1}) \\ & \geq & m_k(T_{d,d-2}) + m_{k-1}(P_{d-3}) \\ & = & m_k(T_{d+1,d-2}). \end{array}$$

**Subcase 2.2** When v lies outside any cycle.

In this case, H contains two cycles  $C_a$  and  $C_b$  with at least one common vertex. Let  $C_a \cdot C_b$  denote the subgraph of G induced by  $V(C_a) \cup V(C_b)$ .

First, suppose that v lies on P(G), say  $v = x_i$ .

If vertices on P(G) lie outside any cycle, then  $H \supseteq C_a \cdot C_b \cup P_i \cup P_{d-i}$ . Thus,

$$m_k(H) \ge m_k(C_a \cdot C_b \cup P_i \cup P_{d-i}) \ge m_k(P_3 \cup P_i \cup P_{d-i}) \ge m_k(P_{d+1}) \ge m_k(T_{d+1,d-2}).$$

Otherwise,  $H \supseteq P_i \cup G_1$ , where  $G_1 \in \mathcal{B}(s_1, d_1)$ ,  $d_1 \ge \max\{d - i - 1, 2\}$  and  $d_1 + 2 \le s_1 \le n - 2 - i$ .

Suppose that  $s_1 \ge d_1 + 3$ . If  $d_1 = 2$ , then  $i \ge d - 3$  and  $s_1 \ge 5$ . Thus we have

$$m_k(H) \ge m_k(P_i \cup G_1) \ge m_k(P_i \cup S_{s_1}) \ge m_k(P_i \cup T_{5,2}) \ge m_k(T_{i+4,i+1}) \ge m_k(T_{d+1,d-2}).$$

If  $d_1 \geq 3$ , then  $d-i-1 \leq d_1$ , which deduces that  $s_1 - d_1 \leq n-2-i-(d-i-1) = n-d-1 < h$ . By the induction hypothesis,  $G_1 \succ B_{s_1,d_1}$ , therefore,

$$m_k(H) \ge m_k(P_i \cup G_1) \ge m_k(P_i \cup B_{s_1,d_1}) \ge m_k(P_i \cup T_{s_1,d_1}) \ge m_k(T_{d+1,d-2}).$$

Now suppose that  $s_1=d_1+2$ . In this case,  $G_1$  is obtained by attaching respectively paths  $P_l(0 \le l \le d_1-2)$  and  $P_{d_1-l-2}$  to the two non-adjacent vertices in  $K_4-e$ . If  $d_1=2$ , then  $i \ge d-3$ . It can be easily checked that  $m_k(K_4-e) \ge m_k(T_{5,2})$ . Thus  $m_k(H) \ge m_k(P_i \cup (K_4-e)) \ge m_k(P_i \cup T_{5,2}) \ge m_k(T_{d+1,d-2})$ . If  $d_1 \ge 3$ , choose an edge  $u_0u_1$  of  $G_1$  such that  $u_0$  and  $u_1$  are both of degree 3 in  $K_4-e$ . Then we get

$$\begin{array}{lll} m_k(H) & \geq & m_k(P_i \cup G_1) \\ & = & m_k(P_i \cup G_1 - u_0 u_1) + m_{k-1}(P_i \cup G_1 - u_0 - u_1) \\ & \geq & m_k(P_i \cup U_{s_1,d_1}) + m_{k-1}(P_i \cup P_{l+1} \cup P_{d_1-l-1}) \\ & \geq & m_k(P_i \cup T_{s_1,d_1}) + m_{k-1}(P_i \cup P_{d_1-1}) \\ & \geq & m_k(P_i \cup T_{d-i+1,d-i-1}) + m_{k-1}(P_i \cup P_{d-i-2}) \\ & \geq & m_k(T_{d,d-2}) + m_{k-1}(P_{d-3}) \\ & = & m_k(T_{d+1,d-2}). \end{array}$$

Next, suppose that v lies outside P(G).

In this case,  $H \supseteq G_2$  or  $H \supseteq C_a \cdot C_b \cup P(G)$ , where  $G_2 \in \mathcal{B}(s,d)$  with  $d+2 \le s \le n-2$ . It is easy to verify that  $m_k(H) \ge m_k(T_{d+1,d-2})$ .

Case 3 If any diametrical path of G contains all pendent vertices in G. We can obtain that  $G \succ B_{n,d}$  by similar arguments as those in Case 3 of Theorem 2.

Consequently, the proof is complete.

Combining Theorems 4.4 and 4.5, we obtain the following main result of this section.

**Theorem 4.6** Let  $G \in \mathcal{B}(n,d)$  with  $n \geq 8$ ,  $3 \leq d \leq n-3$  and  $G \neq B_{n,d}$ . Then  $ME(G) > ME(B_{n,d})$ .

*Proof.* According to Theorems 4.4 and 4.5, we have known that  $G \succ B_{n,d}$ . And then using the increasing property (namely,  $G_1 \succ G_2 \Longrightarrow ME(G_1) > ME(G_2)$ ), we get the result we want.

We will conclude this section by discussing the case d = n - 2. Since any graph G in  $\mathcal{B}(n, n - 2)$  is of the form  $B_n^s$  (as shown in Figure 9), where  $0 \le s \le \lfloor n/2 \rfloor - 2$ . Through simple analysis, we get the following result.

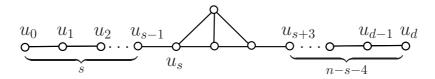


Figure 9: Graph  $B_n^s$  with  $0 \le s \le \lfloor n/2 \rfloor - 2$ .

**Theorem 4.7** Let  $G \in \mathcal{B}(n, n-2)$  with  $n \geq 6$  and  $G \neq B_n^1$ , then  $ME(G) > ME(B_n^1)$ .

*Proof.* Since  $G \in \mathcal{B}(n, n-2)$  and  $G \neq B_n^1$ , then G is  $B_n^s$ , where  $s = 0, 2, \ldots, \lfloor n/2 \rfloor - 2$ .

Case 1  $G = B_n^0$ .

Then  $G - u_d = B_n^0 - u_d = B_n^1 - u_0$  and  $G - u_{d-1} - u_d = B_n^0 - u_{d-1} - u_d > B_n^1 - u_0 - u_1$ . Thus we have  $G = B_n^0 > B_n^1$  by Lemma 2.8.

Case 2  $G = B_n^s(s = 2, ..., \lfloor n/2 \rfloor - 2)$ .

Then

$$m_k(G = B_n^s) = m_k(B_n^s - u_{s-2}u_{s-1}) + m_{k-1}(B_n^s - u_{s-2} - u_{s-1})$$
  
=  $m_k(P_{s-1} \cup B_{n-s+1}^1) + m_{k-1}(P_{s-2} \cup B_{n-s}^0),$ 

together with

$$\begin{array}{lcl} m_k(B_n^1) & = & m_k(B_n^1 - u_{d-s+1}u_{d-s+2}) + m_{k-1}(B_n^1 - u_{d-s+1} - u_{d-s+2}) \\ & = & m_k(P_{s-1} \cup B_{n-s+1}^1) + m_{k-1}(P_{s-2} \cup B_{n-s}^1). \end{array}$$

By Case 1, we have got that  $B_{n-s}^0 \succ B_{n-s}^1$ , then  $m_{k-1}(P_{s-2} \cup B_{n-s}^0) \ge m_{k-1}(P_{s-2} \cup B_{n-s}^1)$  and  $m_2(P_{s-2} \cup B_{n-s}^0) > m_2(P_{s-2} \cup B_{n-s}^1)$ . Thus  $G = B_n^s \succ B_n^1$ .

Therefore, we always have  $G \succ B_n^1$ . And then  $ME(G) > ME(B_n^1)$ .

## 5 Summary

In [25, 35], the authors introduced the concept of "set-complexity", based on a context-dependent measure of information, and used this concept to describe the complexity of gene interaction networks. The binary graphs and edge-colored graphs are studied and the relation between complexity and structure of these graphs is examined in detail. In contrast, we put the emphasis on analyzing properties of spectra-based entropies and study interrelations thereof.

In this paper, we characterize the graphs with minimal matching energy among all unicyclic and bicyclic graphs with a given diameter d. With respect to matching energy of graphs,  $U_{n,d}$  and  $B_{n,d}$  are two extremal graphs in  $\mathcal{U}(n,d)$  and  $\mathcal{B}(n,d)$  respectively. Moreover, both of them are interesting and have the similar extremum property in other aspects. For example, among all unicyclic graphs of a given diameter,  $U_{n,d}$  is the extremal graph on graph energy [29]. Besides, it is also the underling graph of the extremal graph on skew energy [38]. In addition,  $B_{n,d}$  has the minimal energy in one class of bicyclic graphs with a given diameter [39]. From this point, we guess that this two graphs may also be the extremal graphs on some other parameters of graphs. Studying the properties of this two graphs will be one of the future work of us. An important question is how general the bounds are. Obviously, the proof techniques use structural properties of the graphs under consideration and it may be intricate to extend the techniques when using more general graphs. On the other hand, the roots of graph polynomials could be used to characterize graphs structurally. This will be one of the future work. For more results, we refer to [11, 28].

**Acknowledgement.** The authors would like to thank the referees for valuable comments. The authors are supported by NSFC, PCSIRT, China Postdoctoral Science Foundation (2014M551015) and China Scholarship Council.

#### References

- [1] Aihara, J. A new definition of Dewar-type resonance energies. J. Am. Chem. Soc. 1976, 98, 2750–2758.
- [2] Bondy, J.A.; Murty, U.S.R. Graph Theory. Springer: Berlin, 2008.
- [3] Bozkurt, S.B.; Bozkurt, D. Sharp upper bounds for energy and Randić energy. MATCH Commun. Math. Comput. Chem. 2013, 70, 669–680.
- [4] Bozkurt, S.B.; Bozkurt, D. On incidence energy. MATCH Commun. Math. Comput. Chem. 2014, 72, 215–225.

- [5] Bozkurt, S.B.; Gutman, I. Estimating the incidence energy. MATCH Commun. Math. Comput. Chem. 2013, 70, 143–156.
- [6] Chen, L.; Shi, Y. The maximal matching energy of tricyclic graphs. MATCH Commun. Math. Comput. Chem., in press.
- [7] Das, K.C.; Gutman, I.; Cevik, A.S.; Zhou, B. On Laplacian energy. MATCH Commun. Math. Comput. Chem. 2013, 70, 689–696.
- [8] Das, K.C.; Mojallal, S.A. Upper bounds for the energy of graphs. MATCH Commun. Math. Comput. Chem. 2013, 70, 657–662.
- [9] Das, K.C.; Mojallal, S.A.; Gutman, I. Improving McClelland's lower bound for energy. MATCH Commun. Math. Comput. Chem. 2013, 70, 663–668.
- [10] Das, K.C.; Sorgun, S. On Randić energy of graphs. MATCH Commun. Math. Comput. Chem. 2014, 72, 227–238.
- [11] Dehmer, M.; Emmert-Streib, F.; Grabner M. A computational approach to construct a multivariate complete graph invariant. Information Sciences 2014, 260, 200–208.
- [12] Dehmer, M.; Li, X.; Shi, Y. Connections between generalized graph entropies and graph energy. Complexity, in press, DOI: 10.1002/cplx.21539.
- [13] Farrell, E.J. An introduction to matching polynomials. J. Comb. Theory B 1979, 27, 75–86.
- [14] Ghorbani, M.; Faghani, M.; Ashrafi, A.R.; Heidari Rad, S.; Graovac, A. An upper bound for energy of matrices associated to an infinite class of fullerenes. MATCH Commun. Math. Comput. Chem. 2014, 71, 341–354.
- [15] Gutman, I. The energy of a graph. Ber. Math.-Statist. Sekt. Forsch. Graz 1978, 103, 1–22.
- [16] Gutman, I. The energy of a graph: old and new results. In: Algebraic Combinatorics and Applications, Betten, A.; Kohnert, A.; Laue, R.; Wassermann A., Eds., Springer: Berlin, 2001, pp. 196–211.
- [17] Gutman, I.; Li, X.; Zhang, J. Graph energy. In: Analysis of Complex Networks: From Biology to Linguistics, Dehmer, M.; Emmert-Streb F., Eds., Wiley-VCH Verlag: Weinheim, 2009, pp. 145–174.
- [18] Gutman, I.; Milun, M.; Trinajstić, N. Topological definition of delocalisation energy. MATCH Commun. Math. Comput. Chem. 1975, 1, 171–175.

- [19] Gutman, I. Acylclic systems with extremal Hückel  $\pi$ -electron energy. Theor. Chim. Acta 1977, 45, 79–87.
- [20] Gutman, I.; Milun, M.; Trinajstić, N. Graph theory and molecular orbitals 19. Nonparametric resonance energies of arbitrary conjugated systems. J. Am. Chem. Soc. 1977, 99, 1692–1704.
- [21] Gutman, I. The matching polynomial. MATCH Commun. Math. Comput. Chem. 1979, 6, 75–91.
- [22] Gutman, I.; Polansky, O.E. Mathematical concepts in Organic Chemistry. Springer-Verlag: Berlin, 1986.
- [23] Gutman, I.; Wagner, S. The matching energy of a graph. Discrete Appl. Match. 2012, 160, 2177–2187.
- [24] Hou, Y. Unicyclic graphs with minimal energy. J. Math. Chem. 2001, 29, 163–168.
- [25] Ignac, T., Sakhanenko, N., Galas, D. Complexity of networks II: The set complexity of edge-colored graphs, Complexity 2012, 17, 23–36.
- [26] Ji, S.; Li, X.; Shi, Y. Extremal matching energy of bicyclic graphs. MATCH Commun. Math. Comput. Chem. 2013, 70, 697–706.
- [27] Ji, S.; Ma, H. The extremal matching energy of graphs. Ars Combinatoria 2014, 115, 343–355.
- [28] Kraus, V.; Dehmer, M.; Emmert-Streib, F. Probabilistic inequalities for evaluating structural network measures. Information Sciences, in Press, DOI: 10.1016/j.ins.2014.07.018.
- [29] Li, F.; Zhou, B. Minimal energy of unicyclic graphs of a given diameter. J. Math. Chem. 2008, 43, 476–484.
- [30] Li, S.; Yan, W. The matching energy of graphs with given parameters. Discrete Appl. Math. 2014, 162, 415–420.
- [31] Li, X.; Shi, Y.; Gutman, I. Graph Energy. Springer: New York, 2012.
- [32] Li, X., Shi, Y., Wei, M., Li, J. On a conjecture about tricyclic graphs with maximal energy. MATCH Commun. Math. Comput. Chem. 2014, 72, 183–214.
- [33] Mateljevic, M.; Bozin, V.; Gutman, I. Energy of a polynomial and the Coulson integral formula. J. Math. Chem. 2010, 48, 1062–1068.
- [34] Milovanovic, I.Z.; Milovanovic, E.I.; Zakic, A. A short note on graph energy. MATCH Commun. Math. Comput. Chem. 2014, 72, 179–182.

- [35] Sakhanenko, N., Galas, D. Complexity of networks I: The set-complexity of binary graphs, Complexity 2011, 17, 51–64.
- [36] Stevanovic, D.; Milosevic, M.; Hic, P.; Pokorny, M. Proof of a conjecture on distance energy of complete multipartite graphs. MATCH Commun. Math. Comput. Chem. 2013, 70, 157–162.
- [37] Yan, W.; Ye, L. On the minimal energy of trees with a given diameter. Appl. Math. Lett. 2005, 18, 1046–1052.
- [38] Yang, X.; Gong, S.; Xu, G. Minimal skew energy of oriented unicyclic graphs with fixed diameter. J. Inequal. Appl. 2013, 418, 1–11.
- [39] Yang, Y.; Zhou, B. Minimal energy of bicyclic graphs of a given diameter. MATCH Commun. Math. Comput. Chem. 2008, 59, 321–342.
- [40] Zhou, B.; Li, F. On minimal energies of trees of a prescribed diameter. J. Math. Chem. 2006, 39, 465–473.