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On Matching Energy of Bicyclic Graphs

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Abstract The matching energy of a graph was defined as the sum of the absolute values of zeros of its matching polynomial. A bicyclic graph is a connected graph in which the number of edges equals the number of vertices plus one. In this paper, some detailed results on ordering the bicyclic graphs according to their matching energy are obtained.

Keywords Bicyclic graph; matching energy; k-matching
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1 Introduction

All graphs in this paper are finite, simple and undirected. A *matching* in a graph is a set of pairwise non-adjacent edges, and by $m_k(G)$ we denote the number of k-matchings of a graph G. It is both consistent and convenient to define $m_0(G)=1$. Let G be a graph with n vertices. The matching polynomial of the graph G is defined as

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

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For convention, $m_k(G) = 0$ for $k < 0$ and $k > \lfloor n/2 \rfloor$, where $\lfloor \cdot \rfloor$ denotes the floor function. For any graph G, all the zeros of $\alpha(G,x)$ are real-valued and the theory of matching polynomial is well elaborated in [3, 4]. Recently, Gutman and Wagner [8] introduced the matching energy of a graph G, denoted by $ME(G)$ and defined as

$$ME(G) = \frac{2}{\pi} \int_0^{\infty} \frac{1}{x^2} \ln \left[\sum_{k \geq 0} m_k(G) x^{2k} \right] \mathrm{d}x, \tag{1}$$

which coincides with the Coulson-type integral formula for the energy when the graph under consideration is a tree. Meanwhile, as mentioned in [8], the following formula can be also considered as the definition of matching energy.

Let G be a simple graph, and let $\mu_1, \mu_2, \ldots, \mu_n$ be the zeros of its matching polynomial. Then

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

The integral on the right side of (1) is increasing in all the coefficients $m_k(G)$. This means that if two graphs G and G' satisfy $m_k(G) \leq m_k(G')$ for all $k \geq 1$, then $ME(G) \leq ME(G')$. If, in addition, $m_k(G) < m_k(G')$ for at least one k, then $ME(G) < ME(G')$. It then motivates the introduction of a *quasi-order* $\succeq$, defined by

$$G \succeq H \Longleftrightarrow m_k(G) \geq m_k(H), \qquad \text{for all non-negative integers } k.$$

If $G \succeq H$ and there exists some k such that $m_k(G) > m_k(H)$, then we write $G \succ H$. By this, we have $G \succeq H \Rightarrow ME(G) \geq ME(H)$ and $G \succ H \Rightarrow ME(G) > ME(H)$. From this fact, one can readily deduce the extremal graphs for matching energy.

A connected graph with n vertices and n (resp. $n+1$, $n+2$) edges is called *unicyclic* (resp. *bicyclic*, *tricyclic*). In [8], Gutman and Wagner characterized the extremal graphs among all graphs of order n, unicyclic graphs on n vertices with extremal matching energy, and bipartite graphs with n vertices and maximum matching energy. Li and Yan [12] characterized the connected graph with given connectivity (resp. chromatic number) which has maximum matching energy. Recently, Chen and Sheng et al. [1, 2, 10] further investigated unicyclic graphs, bicyclic graphs and tricyclic graphs in terms of matching energy.

Denote by $\mathcal{B}_n$ the set of all connected bicyclic graphs of order n. We now define two special classes of bicyclic graphs. Let $\infty_n(r,s)$ denote the graph obtained by the coalescence of the two end vertices of a path $P_{n-r-s+2}$ with one vertex of two cycles C_r and C_s respectively, and $\theta(r,s,t)$ the graph obtained by fusing two triples of pendent vertices of three paths P_{r+2}, P_{s+2} and P_{t+2} to two vertices, as shown in Figure 1. The distance of two cycles C_r and C_s in G is defined as $d_G(C_r,C_s) = \min\{d_G(x,y) \mid x \in V(C_r), y \in V(C_s)\}$, sometimes written as d_G for short. Note that $d_G(C_r, C_s) = 0$ if C_r and C_s have a common vertex, e.g. for $G = \infty_n(r,s)$ such that $s = n - r + 1$. For any graph $G \in \mathcal{B}_n$, G must contain an induced subgraph in such form of either $\infty_n(r,s)$ or $\theta(r,s,t)$, for some non-negative integers r,s,t. Then the set $\mathcal{B}_n$ can be partitioned into two subsets $\mathcal{B}_n^1$ and $\mathcal{B}_n^2$, where $\mathcal{B}_n^1$ is the set of all bicyclic graphs which contain a subgraph of the form $\infty_n(r,s)$, and $\mathcal{B}_n^2$ is the set of all bicyclic graphs which contain a subgraph of the form $\theta(r,s,t)$.

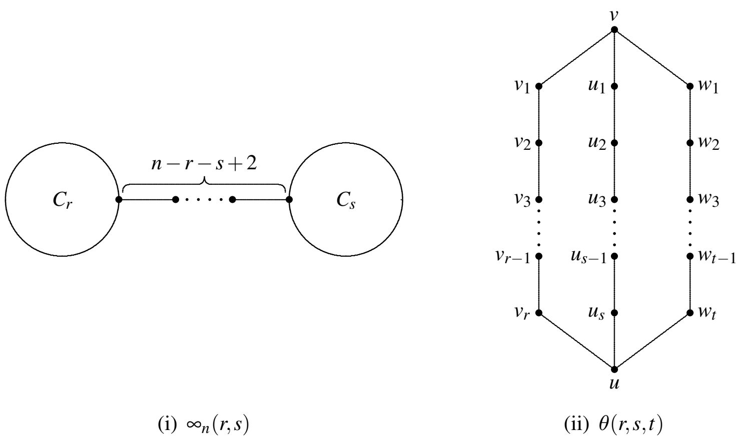

Figure 1.

Ji, Li and Shi [9] characterized the bicyclic graphs with the minimal and maximal matching energy. In this paper, we present some more elaborate results on ordering the bicyclic graphs in terms of their matching energy and consequently the maximum bicyclic graph is obtained.

2 Preliminaries

In this section, we shall present some basic results which will be used in the proof of our main results.

Lemma 2.1 [9] *If u, v are adjacent vertices of G, then for all non-negative integers k,*

$$m_k(G) = m_k(G - uv) + m_{k-1}(G - u - v),$$
$$m_k(G) = m_k(G - v) + \sum_{w \sim v} m_{k-1}(G - v - w),$$

where the sum $\sum_{w \sim v}$ runs over all vertices w adjacent to v.

Consequently, $m_k(G)$ can increase only when edges are added to a graph G and then the following result has been obtained in [8].

Lemma 2.2 [8] *Let G be a graph and e one of its edges. Let $G-e$ be the subgraph obtained by deleting from G the edge e, but keeping all the vertices of G. Then*

$$ME(G-e) < ME(G).$$

Recall the definition of a generalized π-transform in [11]. We say Q is a *branch* of a connected graph G with root u if Q is a connected induced subgraph of G for which u is the only vertex in Q that has a neighbor not in Q. Let P and Q be branches of a component of a graph G with a common root u_0, which is also their only common vertex. Assume that P is a path and u_0 has at least one neighbor in G that does not lie on P or Q. Form a graph from G by relocating the branch Q from u_0 to v where v is the other end vertex of the path P (by deleting edges u_0w and adding new edges vw for every vertex w in Q adjacent to u_0). We refer to the resulting graph as a *generalized π-transform* of G.

Theorem 2.3 [11] *If G' is a generalized π-transform of G, then $G' \succ G$ and so $ME(G') > ME(G)$.*

Note that our result above contains the following [8, Lemma 9] as a special case.

Lemma 2.4 [8] *Suppose that G is a connected graph and T an induced subgraph of G such that T is a tree and T is connected to the rest of G only by a cut vertex v. If T is replaced by a star of the same order, centered at v, then the matching energy decreases (unless T is already such a star). If T is replaced by a path, with one end at v, then the matching energy increases (unless T is already such a path).*

Another transformation concerns reducing the number of pendent paths of a graph. This result had been obtained initially by Gutman [5] and now another proof is given as follows.

Theorem 2.5 *Let G be an arbitrary graph and let u and v be two adjacent vertices with $d_G(u) \geq 2$. If G_1 and G_2 are the graphs obtained from G by inserting t vertices into the edge uv and joining the vertex u to an end vertex of a path P_t, respectively, then $G_1 \succ G_2$.*

Proof. Let the path attached at the vertex u in G_2 be denoted by $P = u_0u_1u_2\cdots u_t$, where u_t is a pendent vertex and u_0 stands for the vertex u. We consider the vertex-sets and edge-sets of G_1 and G_2 to be the same under the obvious correspondence. Particularly, the edge u_tv of G_1 is identified with the edge uv of G_2.

For any k-matching M of G_2, if $uv \notin M$ or $u_{t-1}u_t \notin M$, then the set of edges in G_1 corresponding to M, which we denote by M', is clearly a matching of G_1 (with the same number of edges as M). Let $\mathcal{M}_1$ denote the set of all matchings M' of G_1 obtained in this way. Note that for any $M' \in \mathcal{M}_1$, exactly one of the following holds: the vertex u_t is not covered by M' (which happens when $u_{t-1}u_t \notin M$ and $uv \notin M$), or $u_{t-1}u_t \in M'$ (which happens when $u_{t-1}u_t \in M$ and $uv \notin M$), or $vu_t \in M'$ and u is not covered by M' (which happens when $u_{t-1}u_t \notin M$ and $uv \in M$).

If $u_{t-1}u_t \in M$ and $uv \in M$, then we take M' to be the matching of G_1 which equals $\{u_iu_{i+1} \mid u_{t-i-1}u_{t-i} \in M\}$ on $E(P)$ and agrees with M on $E(G_2) \setminus E(P)$ (but replacing the edge uv by vu_t). Let $\mathcal{M}_2$ denote the set of all matchings M' of G_1 obtained in this way. Note that for any $M' \in \mathcal{M}_2$ we have $vu_t \in M'$ and $u_0u_1 \in M'$.

It is readily checked that $\mathcal{M}_1 \cap \mathcal{M}_2 = \emptyset$ and $\mathcal{M}_1 \cup \mathcal{M}_2$ consists of all matchings M' of G_1 that satisfies (exactly) one of the following: u_t is not covered by M'; $u_{t-1}u_t \in M'$; $vu_t \in M'$ and either u_0 is not covered by M' or $u_0u_1 \in M'$. Moreover, the correspondence $M \mapsto M'$ is a one-to-one mapping from the set of all matchings of G_2 onto $\mathcal{M}_1 \cup \mathcal{M}_2$. This establishes the inequality $m_k(G_1) \geq m_k(G_2)$ for every positive integer k.

Note that a matching M' of G_1 is not in $\mathcal{M}_1 \cup \mathcal{M}_2$ if and only if $vu_t \in M'$, u_0 is covered by M' but $u_0u_1 \notin M'$. If w is a neighbor of u_0 in G_1 other than u_1 – which exists by our assumption on the neighbors of u_0 in G_2 – then clearly $\{vu_t, u_0w\}$ is a 2-matching of G_1 that lies outside $\mathcal{M}_1 \cup \mathcal{M}_2$; hence $m_2(G_1) > m_2(G_2)$. □

Lemma 2.6 [13] *Let $n = 4k, 4k+1, 4k+2$ or $4k+3$. Then*

$$\begin{aligned} P_n &\succ P_2 \cup P_{n-2} \succ P_4 \cup P_{n-4} \succ \cdots \succ P_{2k} \cup P_{n-2k} \succ P_{2k+1} \cup P_{n-2k-1} \\ &\succ P_{2k-1} \cup P_{n-2k+1} \succ \cdots \succ P_3 \cup P_{n-3} \succ P_1 \cup P_{n-1}. \end{aligned}$$

Lemma 2.7 [7] *If $G_1 \succ G_2$, then $G_1 \cup H \succ G_2 \cup H$, where H is an arbitrary graph.*

Applying the lemmas above, we can generalize Lemma 2.6 to the following form, the union of three paths.

Lemma 2.8 *Let r, s, t be non-negative integers with $r \leq s-2$. If r is even, then*

$$P_{r-2} \cup P_{s+2} \cup P_t \succ P_r \cup P_s \cup P_t \succ P_{r+1} \cup P_{s-1} \cup P_t \succ P_{r-1} \cup P_{s+1} \cup P_t.$$

Proof. By Lemma 2.6, we have

$$P_{r-2} \cup P_{s+2} \succ P_r \cup P_s \succ P_{r+1} \cup P_{s-1} \succ P_{r-1} \cup P_{s+1}.$$

By Lemma 2.7 meanwhile, we obtain

$$P_{r-2} \cup P_{s+2} \cup P_t \succ P_r \cup P_s \cup P_t \succ P_{r+1} \cup P_{s-1} \cup P_t \succ P_{r-1} \cup P_{s+1} \cup P_t.$$

□

3 Main results

In this section, the matching energy of bicyclic graphs in respective subclasses is investigated and the ordering of graphs in these subclasses is established.

Any bicyclic graph G can be regarded as obtained from adding some rooted trees on such a graph of the form $\theta(r,s,t)$ or $\infty_n(r,s)$. We know any tree can be transformed into a path by applying a series of generalized π-transforms. By Lemma 2.4, when all such rooted trees are replaced with corresponding paths with the same order, the matching energy of G increases. Meanwhile, by Theorem 2.5, its matching energy increases further when a path is integrated into the cycle. Thus, in terms of discussing maximal matching energy of bicyclic graphs, it suffices to consider the bicyclic graphs of the form $\theta(r,s,t)$ or $\infty_n(r,s)$.

First, we shall establish the ordering of bicyclic graphs of the form $\infty_n(r,n-r+1)$, which contains [5, Lemma 8] as a special case. For the purpose, a result in [11] is listed here, which will be used in the next proof.

Lemma 3.1 [11] *Let m,n be non-negative integers with at least one positive. For any non-negative integer $k \leq (m+n)/2$,*

$$m_k(P_n \cup P_m) = \sum_{l=0}^{r} (-1)^l \binom{n+m-k-l}{k-l}, \tag{2}$$

where $r = \min\{k,m,n\}$.

Theorem 3.2 *Let $n+1 = 4r+s$, where $0 \leq s \leq 3$ and $r \geq 2$. Then*

$$\begin{aligned}
&\infty_n(4,n-3) \succ \infty_n(6,n-5) \succ \cdots \succ \infty_n(2r,2r+s) \\
&\qquad \succ \infty_n(2r-1,2r+s+1) \succ \cdots \succ \infty_n(5,n-4) \succ \infty_n(3,n-2).
\end{aligned}$$

Proof. Consider the bicyclic graph $G = \infty_n(p,q)$ on $n = p+q-1$ vertices. Without loss of generality, assume that $p \geq q$. Set $G_1 = \infty_n(p+1,q-1)$ and $G_2 = \infty_n(p+2,q-2)$. Assume that the common vertex of two cycles in G (resp. G_1, G_2) is v (resp. v', v'').

By Lemma 2.1, we have

$$\begin{aligned}
m_k(G) &= m_k(G-v) + \sum_{u \sim v} m_{k-1}(G-v-u) \\
&= m_k(P_{p-1} \cup P_{q-1}) + 2m_{k-1}(P_{p-2} \cup P_{q-1}) + 2m_{k-1}(P_{p-1} \cup P_{q-2}); \\
m_k(G_1) &= m_k(G_1-v') + \sum_{u \sim v'} m_{k-1}(G_1-v'-u) \\
&= m_k(P_p \cup P_{q-2}) + 2m_{k-1}(P_p \cup P_{q-3}) + 2m_{k-1}(P_{p-1} \cup P_{q-2}); \\
m_k(G_2) &= m_k(G_2-v'') + \sum_{u \sim v''} m_{k-1}(G-v''-u) \\
&= m_k(P_{p+1} \cup P_{q-3}) + 2m_{k-1}(P_{p+1} \cup P_{q-4}) + 2m_{k-1}(P_p \cup P_{q-3}).
\end{aligned}$$

Next we shall discuss the variation of k-matching numbers of G_1 and G_2 perturbed from the graph G. First, consider what happens to G_1 in terms of the number of k-matchings for any k. Applying Lemma 3.1, we have

$$\begin{aligned}
&m_k(G)-m_k(G_1)\\
&=m_k(P_{p-1}\cup P_{q-1})+2m_{k-1}(P_{p-2}\cup P_{q-1})-m_k(P_p\cup P_{q-2})-2m_{k-1}(P_p\cup P_{q-3})\\
&=\sum_{l=0}^{r_3}(-1)^l\binom{p+q-k-l-2}{k-l}+2\sum_{l=0}^{r_4}(-1)^l\binom{p+q-k-l-2}{k-l-1}\\
&\quad-\sum_{l=0}^{r_1}(-1)^l\binom{p+q-k-l-2}{k-l}-2\sum_{l=0}^{r_2}(-1)^l\binom{p+q-k-l-2}{k-l-1},
\end{aligned}$$

where $r_1=\min\{k,q-2,p\}$, $r_2=\min\{k-1,q-3,p\}$, $r_3=\min\{k,q-1,p-1\}$, $r_4=\min\{k-1,q-1,p-2\}$. We shall distinguish it in three cases according to the value of k.

Case 1. $k\le q-2$. In this case, it is easy to see that $r_1=r_3=k$ and $r_2=r_4=k-1$. Thus $m_k(G)-m_k(G_1)=0$.

Case 2. $k=q-1$. In this case, $r_1=r_3-1=q-2$ and $r_2=r_4-1=q-3$. By a straight calculation, we have

$$\begin{aligned}
&m_k(G)-m_k(G_1)\\
&=(-1)^{q-1}\binom{p+q-k-(q-1)-2}{k-(q-1)}+2(-1)^{q-2}\binom{p+q-k-(q-2)-2}{k-(q-2)-1}\\
&=(-1)^{q-1}+2(-1)^{q-2}\\
&=(-1)^q.
\end{aligned}$$

Case 3. $k\ge q$. Note that then $r_1=r_3-1=q-2$, $r_2=q-3$ and either $r_4=q-2$ when $p=q$ or $r_4=q-1$ when $p>q$. Thus if $p>q$, we have

$$\begin{aligned}
&m_k(G)-m_k(G_1)\\
&=(-1)^{q-1}\binom{p+q-k-(q-1)-2}{k-(q-1)}+2(-1)^{q-1}\binom{p+q-k-(q-1)-2}{k-(q-1)-1}\\
&\quad+2(-1)^{q-2}\binom{p+q-k-(q-2)-2}{k-(q-2)-1)}\\
&=(-1)^{q-1}\binom{p-k-1}{k-q+1}+2(-1)^{q-1}\binom{p-k-1}{k-q}-2(-1)^{q-1}\binom{p-k}{k-q+1}\\
&=(-1)^q\left[2\binom{p-k}{k-q+1}-\binom{p-k-1}{k-q+1}-2\binom{p-k-1}{k-q}\right]\\
&=(-1)^q\binom{p-k-1}{k-q+1};
\end{aligned}$$

and if $p=q$, we have $m_k(G)=m_k(G_1)=0$ because the matching number (the size of maximum matching) of a graph on n vertices is not more than $\lfloor n/2 \rfloor$ while $\lfloor \frac{2q-1}{2} \rfloor = q-1 < q \le k$.

From the cases discussed above, it follows immediately that for any k, $m_k(G)-m_k(G_1)$ is $(-1)^q$ times a non-negative integer which is not identically zero (at least for the case of $k=q-1$). Therefore, we obtain that $\infty_n(p,q) \succ \infty_n(p+1,q-1)$ if q is even and $\infty_n(p+1,q-1) \succ \infty_n(p,q)$ if q is odd.

Finally, we shall show how k-matchings number of G_2 changes in a similar manner, which enables us to know what happens to k-matchings number of a graph $\infty_n(p,q)$ when perturbed while the parity of the length of the shorter cycle keeps unchanged. Note that

$$\begin{aligned}
& m_k(G)-m_k(G_2) \\
&= m_k(P_{q-1}\cup P_{p-1})+2m_{k-1}(P_{q-2}\cup P_{p-1})+2m_{k-1}(P_{q-1}\cup P_{p-2}) \\
&\quad - m_k(P_{q-3}\cup P_{p+1})-2m_{k-1}(P_{q-4}\cup P_{p+1})-2m_{k-1}(P_{q-3}\cup P_{p}) \\
&= \sum_{l=0}^{r_4}(-1)^l\binom{p+q-k-l-2}{k-l}+2\sum_{l=0}^{r_5}(-1)^l\binom{p+q-k-l-2}{k-l-1} \\
&\quad +2\sum_{l=0}^{r_6}(-1)^l\binom{p+q-k-l-2}{k-l-1}-\sum_{l=0}^{r_1}(-1)^l\binom{p+q-k-l-2}{k-l} \\
&\quad -2\sum_{l=0}^{r_2}(-1)^l\binom{p+q-k-l-2}{k-l-1}-2\sum_{l=0}^{r_3}(-1)^l\binom{p+q-k-l-2}{k-l-1},
\end{aligned}$$

where $r_1=\min\{k,q-3,p+1\}$, $r_2=\min\{k-1,q-4,p+1\}$, $r_3=\min\{k-1,q-3,p\}$, $r_4=\min\{k,q-1,p-1\}$, $r_5=\min\{k-1,q-2,p-1\}$, $r_6=\min\{k-1,q-1,p-2\}$. We also distinguish it in cases according to the value of k.

Case 1. $k \le q-3$. In this case, it is easy to see that $r_1=r_4$, $r_2=r_5$ and $r_3=r_6$. So $m_k(G)-m_k(G_2)=0$.

Case 2. $k=q-2$. Then $r_1=r_4-1=q-3$, $r_2=r_5-1=q-4$ and $r_3=r_6=q-3$. Thus

$$\begin{aligned}
& m_k(G)-m_k(G_2) \\
&= (-1)^{q-2}\binom{p+q-k-(q-2)-2}{k-(q-2)}+2(-1)^{q-3}\binom{p+q-k-(q-3)-2}{k-(q-3)-1} \\
&= (-1)^{q-2}-2(-1)^{q-2} \\
&= (-1)^{q-1}.
\end{aligned}$$

Case 3. $k=q-1$. Then $r_1=r_4-2=q-3$, $r_2=r_5-2=q-4$ and $r_3=r_6-1=q-3$.

Thus

$$\begin{aligned}
&m_k(G)-m_k(G_2)\\
&=(-1)^{q-1}\binom{p+q-k-(q-1)-2}{k-(q-1)}+(-1)^{q-2}\binom{p+q-k-(q-2)-2}{k-(q-2)}\\
&\qquad+4(-1)^{q-2}\binom{p+q-k-(q-2)-2}{k-(q-2)-1}+2(-1)^{q-3}\binom{p+q-k-(q-3)-2}{k-(q-3)-1}\\
&=(-1)^{q-1}+(-1)^{q-2}(p-q+1)+4(-1)^{q-2}+2(-1)^{q-3}(p-q+2)\\
&=(p-q)(-1)^{q-1}.
\end{aligned}$$

Case 4. $k\geq q$. Then $r_1=r_4-2=q-3$, $r_2=r_5-2=q-4$, $r_3=q-3$ and either $r_6=q-2$ if $p=q$ or $r_6=q-1$ if $p>q$. Thus if $p>q$, we have

$$\begin{aligned}
&m_k(G)-m_k(G_2)\\
&=(-1)^{q-1}\binom{p+q-k-(q-1)-2}{k-(q-1)}+(-1)^{q-2}\binom{p+q-k-(q-2)-2}{k-(q-2)}\\
&\qquad+2(-1)^{q-2}\binom{p+q-k-(q-2)-2}{k-(q-2)-1}+2(-1)^{q-3}\binom{p+q-k-(q-3)-2}{k-(q-3)-1}\\
&\qquad+2(-1)^{q-1}\binom{p+q-k-(q-1)-2}{k-(q-1)-1}+2(-1)^{q-2}\binom{p+q-k-(q-2)-2}{k-(q-2)-1}\\
&=(-1)^{q-1}\left[2\binom{p-k}{k-q+2}-2\binom{p-k-1}{k-q+1}-\binom{p-k-1}{k-q+2}\right]\\
&=(-1)^{q-1}\binom{p-k-1}{k-q+2};
\end{aligned}$$

and if $p=q$, we have $m_k(G)=m_k(G_2)=0$ because, as mentioned before, the matching number of a graph on n vertices is not more than $\lfloor n/2\rfloor$.

From the arguments above, we have that $\infty_n(p,q)\succ\infty_n(p+2,q-2)$ if q is odd and $\infty_n(p+2,q-2)\succ\infty_n(p,q)$ if q is even. $\square$

Further, the graph in $\mathcal{B}_n^1$ with maximum matching energy is obtained in the following.

Theorem 3.3 *For any $G\in\mathcal{B}_n^1$ with $n\geq 8$, $\infty_n(4,n-4)\succeq G$ with equality holding if and only if $G\cong\infty_n(4,n-4)$.*

Proof. Without loss of generality, assume $G\in\mathcal{B}_n^1$ is of the form $\infty_n(p,q)$. We distinguish it according to the value of d_G, the distance between the cycles C_p and C_q in G.

Case 1. $d_G\geq 1$. Choose two edges u_1u_2 and v_1v_2 in the cycles C_p and C_q of G, respectively, with the degrees of both u_1 and v_1 being 3. Meanwhile, denote by $u_1'v_1'$ the unique edge between the cycles C_4 and C_{n-4} of $\infty_n(4,n-4)$, and $u'_1u'_2$ (resp. $v'_1v'_2$) an edge in the cycle C_4 (resp. C_{n-4}) of $\infty_n(4,n-4)$.

For convenience, let $G=\infty_n(p,q)$ $(p\ge q)$, $G'=\infty_n(4,n-4)$ and $r=n-p-q$. By Lemma 2.1, we have

$$\begin{aligned}m_k(G) &= m_k(G-u_1u_2)+m_{k-1}(G-u_1-u_2)\\ &= m_k(G-u_1u_2-v_1v_2)+m_{k-1}(G-u_1u_2-v_1-v_2)\\ &\quad +m_{k-1}(G-u_1-u_2-v_1v_2)+m_{k-2}(G-u_1-u_2-v_1-v_2)\\ &= m_k(P_n)+m_{k-1}(P_{p+r}\cup P_{q-2})\\ &\quad +m_{k-1}(P_{q+r}\cup P_{p-2})+m_{k-2}(P_{q-2}\cup P_r\cup P_{p-2})\end{aligned}$$

and

$$\begin{aligned}m_k(G') &= m_k(G'-u'_1u'_2)+m_{k-1}(G'-u'_1-u'_2)\\ &= m_k(G'-u'_1u'_2-v'_1v'_2)+m_{k-1}(G'-u'_1u'_2-v'_1-v'_2)\\ &\quad +m_{k-1}(G'-u'_1-u'_2-v'_1v'_2)+m_{k-2}(G'-u'_1-u'_2-v'_1-v'_2)\\ &= m_k(P_n)+m_{k-1}(P_4\cup P_{n-6})+m_{k-1}(P_2\cup P_{n-4})+m_{k-2}(P_2\cup P_{n-6}).\end{aligned} \tag{3}$$

Thus

$$\begin{aligned}m_k(G')-m_k(G) &= m_{k-1}(P_4\cup P_{n-6})+m_{k-1}(P_2\cup P_{n-4})\\ &\quad +m_{k-2}(P_2\cup P_{n-6})-m_{k-1}(P_{p+r}\cup P_{q-2})\\ &\quad -m_{k-1}(P_{q+r}\cup P_{p-2})-m_{k-2}(P_{q-2}\cup P_r\cup P_{p-2}).\end{aligned}$$

When $p\ne 4$, by Lemma 2.6, we have

$$\begin{aligned}&P_2\cup P_{n-4}\succeq P_{p+r}\cup P_{q-2},\\ &P_4\cup P_{n-6}\succeq P_{q+r}\cup P_{p-2},\\ &P_2\cup P_{n-6}\succeq P_{q-2}\cup P_r\cup P_{p-2}.\end{aligned} \tag{4}$$

This implies that for all k,

$$\begin{aligned}&m_{k-1}(P_2\cup P_{n-4})\ge m_{k-1}(P_{p+r}\cup P_{q-2}),\\ &m_{k-1}(P_4\cup P_{n-6})\ge m_{k-1}(P_{q+r}\cup P_{p-2}),\\ &m_{k-2}(P_2\cup P_{n-6})\ge m_{k-2}(P_{q-2}\cup P_r\cup P_{p-2}).\end{aligned}$$

Thus $m_k(G')-m_k(G)\ge 0$ for all k, and the equality holds for all k if and only if all the inequalities above become equalities for all k. By Lemma 2.6, it follows that $P_2\cup P_{n-4}\cong P_{p+r}\cup P_{q-2}$, $P_4\cup P_{n-6}\cong P_{q+r}\cup P_{p-2}$ and $P_2\cup P_{n-6}\cong P_{q-2}\cup P_r\cup P_{p-2}$. The first one holds if and only if $q=4$ and in this case the last one holds if and only if $r=0$. As a result, the middle one holds also. Therefore, $G' \succeq G$ and $G \cong G'$ if and only if $q = 4$ and $r = 0$, namely $G \cong \infty_n(4, n-4) = G'$.

When $p = 4$, then $q = 3, 4$ due to $p \geq q \geq 3$.

If $q = 3$, then

$$\begin{aligned} m_k(G') - m_k(G) &= m_{k-1}(P_4 \cup P_{n-6}) + m_{k-1}(P_2 \cup P_{n-4}) \\ &\quad + m_{k-2}(P_2 \cup P_{n-6}) - m_{k-1}(P_1 \cup P_{n-3}) \\ &\quad - m_{k-1}(P_2 \cup P_{n-4}) - m_{k-2}(P_1 \cup P_2 \cup P_{n-7}) \\ &= m_{k-1}(P_4 \cup P_{n-6}) - m_{k-1}(P_1 \cup P_{n-3}) \\ &\quad + m_{k-2}(P_2 \cup P_{n-6}) - m_{k-2}(P_1 \cup P_2 \cup P_{n-7}). \end{aligned}$$

Because $P_4 \cup P_{n-6} \succ P_1 \cup P_{n-3}$ and $P_2 \cup P_{n-6} \succ P_1 \cup P_2 \cup P_{n-7}$, we have $G' \succ G$.

Now assume that $q = 4$. If $n = 8$, obviously $G \cong \infty_8(4, 4) = G'$. If $n \geq 9$, we have

$$\begin{aligned} m_k(G') - m_k(G) &= m_{k-1}(P_4 \cup P_{n-6}) + m_{k-1}(P_2 \cup P_{n-4}) \\ &\quad + m_{k-2}(P_2 \cup P_{n-6}) - m_{k-1}(P_2 \cup P_{n-4}) \\ &\quad - m_{k-1}(P_2 \cup P_{n-4}) - m_{k-2}(P_2 \cup P_2 \cup P_{n-8}) \\ &= m_{k-1}(P_4 \cup P_{n-6}) + m_{k-2}(P_2 \cup P_{n-6}) \\ &\quad - m_{k-1}(P_2 \cup P_{n-4}) - m_{k-2}(P_2 \cup P_2 \cup P_{n-8}) \\ &= m_{k-1}(P_2 \cup P_2 \cup P_{n-6}) + m_{k-2}(P_{n-6}) + m_{k-2}(P_2 \cup P_2 \cup P_{n-8}) \\ &\quad + m_{k-3}(P_2 \cup P_{n-9}) - m_{k-1}(P_2 \cup P_2 \cup P_{n-6}) \\ &\quad - m_{k-2}(P_2 \cup P_{n-7}) - m_{k-2}(P_2 \cup P_2 \cup P_{n-8}) \\ &= m_{k-2}(P_{n-6}) + m_{k-3}(P_2 \cup P_{n-9}) \\ &\quad - m_{k-2}(P_2 \cup P_{n-8}) - m_{k-3}(P_2 \cup P_{n-9}) \\ &= m_{k-2}(P_{n-6}) - m_{k-2}(P_2 \cup P_{n-8}) \\ &= m_{k-3}(P_{n-9}). \end{aligned}$$

Note that $m_{k-3}(P_{n-9}) \geq 0$ for all k and the inequality holds strictly at least for $k = 3$ as $m_0(P_{n-9}) = 1$. This means that $G' \succ G$ in this case.

Therefore, in the case of $d_G \geq 1$, $G' \succeq G$ with equality holding if and only if $G \cong G'$.

Case 2. $d_G = 0$. By the same way, consider $\infty_n(p, q)$ with $p + q = n + 1$ and by Lemma 2.1, we have

$$m_k(\infty_n(p, q)) = m_k(P_n) + m_{k-1}(P_{p-1} \cup P_{q-2}) + m_{k-1}(P_{p-2} \cup P_{q-1}).$$

Then together with the expression (3) of $m_k(\infty_n(4,n-4))$, we get

$$\begin{aligned} m_k(\infty_n(4,n-4)) - m_k(\infty_n(p,q)) &= m_{k-1}(P_4 \cup P_{n-6}) + m_{k-1}(P_2 \cup P_{n-4}) \\ &\quad + m_{k-2}(P_2 \cup P_{n-6}) - m_{k-1}(P_{p-1} \cup P_{q-2}) \\ &\quad - m_{k-1}(P_{p-2} \cup P_{q-1}) \\ &\geq m_{k-2}(P_2 \cup P_{n-6}), \end{aligned}$$

where the last inequality can be proved easily by Lemma 2.6. Obviously $\infty_n(4,n-4) \succ \infty_n(p,q)$ in this case since there exists at least a strict inequality. $\square$

Finally, we tend to establish the ordering of bicyclic graphs in the second class $\mathcal{B}_n^2$, of which the result [5, Lemma 9] is a special case.

Theorem 3.4 *For any bicyclic graph $G \in \mathcal{B}_n^2$ with $n \geq 5$,*

$$ME(G) \leq ME(\theta(0,2,n-4)),$$

with equality if and only if $G \cong \theta(0,2,n-4)$. More precisely, if r,s,t are integers with $t = \max\{r,s,t\}$, then

(a) if $s \geq 2$, r is even and $r \leq t-2$, then

$$\theta(r-2,s,t+2) \succ \theta(r,s,t) \succ \theta(r+1,s,t-1) \succ \theta(r-1,s,t+1). \tag{5}$$

(b) $\theta(0,2,n-4) \succ \theta(r,s,t)$ for $s = 0,1$.

Proof. Let G be an arbitrary graph chosen from $\mathcal{B}_n^2$. Without loss of generality, assume that G is of the form $\theta(r,s,t)$, which can be viewed as obtained by fusing two triples of pendent vertices v_0,u_0,w_0 and v_{r+1},u_{s+1},w_{t+1} of three paths $P_{r+2} = v_0v_1\cdots v_rv_{r+1}$, $P_{s+2} = u_0u_1\cdots u_su_{s+1}$ and $P_{t+2} = w_0w_1\cdots w_tw_{t+1}$ to two vertices, say v and u, respectively. By Lemma 2.1, we have

$$\begin{aligned} m_k(G) &= m_k(G-vu_1) + m_{k-1}(G-v-u_1) \\ &= m_k(G-vu_1-uu_s) + m_{k-1}(G-vu_1-u-u_s) \\ &\quad + m_{k-1}(G-v-u_1-uu_s) + m_{k-2}(G-v-u_1-u-u_s) \\ &= m_k(P_s \cup C_{r+t+2}) + 2m_{k-1}(P_{s-1} \cup P_{r+t+1}) + m_{k-2}(P_{s-2} \cup P_r \cup P_t). \end{aligned}$$

By Lemma 2.8, it follows directly that if $s-2 \geq 0$ and r is even, then

$$P_{s-2} \cup P_{r-2} \cup P_{t+2} \succ P_{s-2} \cup P_r \cup P_t \succ P_{s-2} \cup P_{r+1} \cup P_{t-1} \succ P_{s-2} \cup P_{r-1} \cup P_{t+1}$$

and so the assertion (5) holds.

Now consider the graphs $\theta(r,s,t)$ for the cases of $s \leq 1$. For convenience, let $G_3 = \theta(r,1,t)$ and $G_4 = \theta(r',0,t')$ with $G_4 \neq \theta(0,2,n-4)$. Suppose that vu_1u is one of three paths in G_3, with the degrees of v and u being 3. Similarly, let $v'u'$ be the edge in G_4 with $d(v') = d(u') = 3$. By Lemma 2.1, we have

$$\begin{aligned} m_k(G_3) &= m_k(G_3 - u_1) + m_{k-1}(G_3 - u_1 - v) + m_{k-1}(G_3 - u_1 - u) \\ &= m_k(C_{n-1}) + 2m_{k-1}(P_{n-2}) \\ &= m_k(P_{n-1}) + m_{k-1}(P_{n-3}) + 2m_{k-1}(P_{n-2}), \\ m_k(G_4) &= m_k(G_4 - v'u') + m_{k-1}(G_4 - v' - u') \\ &= m_k(C_n) + m_{k-1}(P_{r'} \cup P_{t'}) \\ &= m_k(P_{n-1}) + 2m_{k-1}(P_{n-2}) + m_{k-1}(P_{r'} \cup P_{t'}). \end{aligned}$$

It is easy to note that $G_4 \succ G_3$ because $m_k(G_4) - m_k(G_3) = m_{k-1}(P_{r'} \cup P_{t'}) - m_{k-1}(P_{n-3}) \geq 0$ for all $k \geq 1$ as by Lemma 2.6, $P_{r'} \cup P_{t'} \succ P_{n-3} \cup P_1$, where $r' + t' = n-2$. Further, the assertion (b) can be completed once $\theta(0,2,n-4) \succ G_4$ $(= \theta(r',0,t'))$ holds. Set $H = \theta(0,2,n-4)$ for convenience. Assume that vu_1u_2u is the path in H with $d(v) = d(u) = 3$. By Lemma 2.1, we have

$$\begin{aligned} m_k(H) &= m_k(H - uv) + m_{k-1}(H - u - v) \\ &= m_k(H - uv - u_1u_2) + m_{k-1}(H - uv - u_1 - u_2) + m_{k-1}(H - u - v) \\ &= m_k(P_n) + m_{k-1}(P_{n-2}) + m_{k-1}(P_2 \cup P_{n-4}) \\ &= m_k(P_{n-1}) + 2m_{k-1}(P_{n-2}) + m_{k-1}(P_2 \cup P_{n-4}). \end{aligned}$$

So

$$m_k(H) - m_k(G_4) = m_{k-1}(P_2 \cup P_{n-4}) - m_{k-1}(P_{r'} \cup P_{t'}).$$

Therefore $H \succ G_4$ since $P_2 \cup P_{n-4} \succ P_{r'} \cup P_{t'}$ by Lemma 2.6.

Combining two arguments above, it follows immediately that for any $G \in \mathcal{B}_n^2$, $\theta(0,2,n-4) \succeq G$, with equality if and only if $G \cong \theta(0,2,n-4)$, and so the main result holds. $\square$

Theorem 3.5 [9] *$ME(\theta(0,2,n-4)) < ME(\infty_n(4,n-4))$ for $n \geq 10$ and $n = 8$, exceptionally $ME(\theta(0,2,n-4)) = ME(\infty_n(4,n-4))$ for $n = 9$.*

From Theorems 3.3 and 3.4, we know that the maximal graphs in $\mathcal{B}_n^1$ and $\mathcal{B}_n^2$ are $\infty_n(4,n-4)$ and $\theta(0,2,n-4)$ respectively. Meanwhile by Theorem 3.5, we conclude with the following result, which can also be found in [9].

Theorem 3.6 *Let $G \in \mathcal{B}_n$ with $n \geq 10$ and $n = 8$. Then $ME(G) \leq ME(\infty_n(4,n-4))$, with equality if and only if $G \cong \infty_n(4,n-4)$. Exceptionally, when $n = 9$, $\infty_n(4,n-4)$ and $\theta(0,2,n-4)$ have equivalent matching energy and both are maximal graphs in $\mathcal{B}_n$.*

References

[1] L. Chen, Y. Shi, The maximal matching energy of tricyclic graphs, *MATCH Commun. Math. Comput. Chem.* 73 (2015) 105–119.

[2] L. Chen, J. Liu, Y. Shi, Matching energy of unicyclic and bicyclic graphs with a given diameter, *Complexity*, in press.

[3] D. M. Cvetković, M. Doob, I. Gutman, A. Torgašev, Recent Results in the Theory of Graph Spectra, North-Holland, Amsterdam, 1988.

[4] I. Gutman, The matching polynomial, *MATCH Commun. Math. Comput. Chem.* 6 (1979) 75–91.

[5] I. Gutman, Graphs with greatest number of matchings, *Publ. Inst. Math. (Beograd)* 27 (1980) 67–76.

[6] I. Gutman, Correction of the paper "Graphs with greatest number of matchings", *Publ. Inst. Math. (Beograd)* 32 (1982) 61–63.

[7] I. Gutman, D. Cvetković, Finding tricyclic graphs with a maximal number of matchings - another example of computer aided research in graph theory, *Publ. Inst. Math. (Beograd)* 35 (1984) 33–40.

[8] I. Gutman, S. Wagner, The matching energy of a graph, *Discrete Appl. Math.* 160 (2012) 2177–2187.

[9] S. Ji, X. Li, Y. Shi, Extremal matching energy of bicyclic graphs, *MATCH Commun. Math. Comput. Chem.* 70 (2013) 697–706.

[10] S. Ji, H. Ma, The extremal matching energy of graphs, *Ars Combin.* 115 (2014) 343–355.

[11] H.-H. Li, B.-S. Tam, L. Su, On the signless Laplacian coeffcients of unicyclic graphs, *Linear Algebra Appl.* 439 (2013) 2008–2028.

[12] S. Li, W. Yan, The matching energy of graphs with given parameters, *Discrete Appl. Math.* 162 (2014) 415–420.

[13] X. Li, Y. Shi, I. Gutman, Graph Energy, Springer, New York, 2012.