Extremal Matching Energy of Bicyclic Graphs*

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Abstract

The energy of a graph G is equal to the sum of the absolute values of the eigenvalues of G. Recently, Gutman and Wagner proposed the concept of the 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 is defined as the sum $\sum_{i=0}^{n} |\mu_i|$. In this paper, we characterize the graphs with the extremal matching energy among all bicyclic graphs, and completely determine the graphs with the minimal and maximal matching energy in bicyclic graphs.

1 Introduction

In this paper, the graphs under our consideration are finite, connected, undirected and simple. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of a graph G. The energy of graph G [4] is defined as

$$E(G) = \sum_{i=0}^{n} |\lambda_i| \ .$$

A *matching* in a graph G is a set of pairwise nonadjacent edges. A matching M is called k-*matching* if the size of M is k. Let $m(G,k)$ denote the number of k-matchings of G,

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where $m(G,1)=m$, and $m(G,k)=0$ for $k>\frac{n}{2}$. In addition, $m(G,0)=1$. The matching polynomial of the graph G is defined as

$$\alpha(G)=\alpha(G,\lambda)=\sum_{k\geq 0}(-1)^k\, m(G,\lambda)\, \lambda^{2k}\ .$$

An important tool of graph energy is the Coulson integral formula [4] (with regard to G be a tree T):

$$E(G)=\frac{2}{\pi}\int_0^{+\infty}\frac{1}{x^2}\ln\left[\sum_{k\geq 0} m(T,k)\, x^{2k}\right]dx\ . \tag{1.1}$$

The theory of graph energy is well developed. Moreover, it has been rather widely concerned by theoretical chemists and mathematicians. For details see the new book on graph energy [18] and the reviews [8, 10].

Recently, Gutman and Wagner [13] proposed the matching–energy concept. (In addition, energy and matching energy are closely related, and they are two quantities of relevance for chemical applications; for details see [1, 11, 12].)

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

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

In view of Eq. (1.1), the matching energy also has a beautiful formula as follows.

Proposition 1.2 *Let G be a graph of order n, and let $m(G,k)$ be the number of its $k-$matchings, $k=0,1,2,\ldots,\lfloor n/2\rfloor$. The matching energy of G is the given by*

$$ME=ME(G)=\frac{2}{\pi}\int_0^{+\infty}\frac{1}{x^2}\ln\left[\sum_{k\geq 0} m(G,k)\, x^{2k}\right]dx\ . \tag{1.2}$$

By Formula (1.2) and the monotony of the function logarithm, we can define a *quasi-order* as follows: If two graphs G_1 and G_2 have the same order and size, then

$$m(G_1,k)\preceq m(G_2,k) \qquad \text{for} \;\; 1\leq k\leq \lfloor n/2\rfloor \Longleftrightarrow ME(G_1)\leq ME(G_2)\ .$$

We now introduce some elementary notations and terminologies that will be used in the sequel. With regard to other notations, the readers are referred to the book [2]. Let $\mathscr{U}_n$ denote the set of all connected unicyclic graphs of order n. Let P_n^{ℓ} be the graph obtained by attaching a vertex of C_ℓ and a pendent vertex of $P_{n-\ell+1}$.

Denote by $\mathscr{B}_n$ the set of all connected bicyclic graphs of order n. We now define two special classes graphs. Let $P_n^{k,\ell}$ be the graph obtained by connecting two cycles C_k and C_ℓ with a path $P_{n-k-\ell}$, and $C_n(\ell, r, t)$ be the graph obtained by fusing two triples of pendent vertices of three paths $P_{\ell+1}$, P_{r+1} and P_{t+1} to two vertices. (Without loss of generality, we set $1 \leq r \leq \ell \leq t$.) The distance of C_1 and C_2 of the graph G is defined as $d_G(C_1, C_2) = min\{d(x, y)|x \in V(C_1), y \in V(C_2)\}$. (For simplicity, we write d_G), the corresponding path is marked by xTy. If C_1 and C_2 have a common vertex, then $d_G(C_1, C_2) = 0$. Let G be a graph in $\mathscr{B}_n$. If G contains $C_s(\ell, r, t)$ or $P_s^{\ell,r}$ as its subgraph, then we call them as a *brace* of G, respectively. By this way, bicyclic graphs can be partitioned into two subsets $\mathscr{B}_n^1$ and $\mathscr{B}_n^2$, where $\mathscr{B}_n^1$ is the set of all bicyclic graphs which includes $C_s(\ell, r, t)$ as its brace, and $\mathscr{B}_n^2$ is the set of all bicyclic graph which contains $P_s^{\ell,r}$ as its brace.

As the research of extremal graph energy is an amusing work (for some newest literature see [14–17]), the study on extremal matching energy is also interesting. In [13], the authors gave some elementary results on the matching energy and obtained that $ME(T) = E(T)$ for any tree T, and $ME(S_n^+) \leq ME(G) \leq ME(C_n)$ for any unicyclic graph G, where S_n^+ is the graph obtained by adding a new edge to the star S_n . In the paper, we characterize the graphs with the extremal matching energy among all bicyclic graphs, and completely determine the bicyclic graphs with minimal and the maximal matching energy.

In the 1980s, Gutman determined the unicyclic [6], bicyclic [7], and tricyclic [9] graphs with maximal matchings, i.e., graphs that are extremal with regard to the quasi-ordering $\preceq$. From these results, using Eq. (1.2), the finding of unicyclic, bicyclic, and tricyclic graphs with maximal matching energy is an elementary task. The results reported in the present paper were obtained without knowledge of [6,7,9]. We learned about these papers from the referee.

Theorem 1.3 *Let $G \in \mathscr{B}_n$ with $n \geq 10$ and $n = 8$. Then $ME(S_n^*) \leq ME(G) \leq ME(P_n^{4,n-4})$, with equality if and only if $G \cong S_n^*$ and $G \cong P_n^{4,n-4}$, where S_n^* denotes the graph obtained by joining one pendent vertex of S_n to its other two pendent vertices, respectively. Exceptionally, when $n = 9$, $P_n^{4,n-4}$ and $C_n(3, 1, n-3)$ are matching–equivalent and thus both have maximal ME-values.*

2 Preliminary

In [3, 5], we have two fundamental identities as the following proposition.

Proposition 2.1 *Let G be a graph. Then, for any edge e=uv and $N(u) = \{v_1(= v), v_2, \ldots, v_t\}$, we have the two identities:*

$$m(G, k) = m(G - uv, k) + m(G - u - v, k - 1) \tag{2.1}$$

$$m(G, k) = m(G - u, k) + \sum_{i=0}^{|N(u)|} m(G - u - v_i, k - 1) \ . \tag{2.2}$$

Lemma 2.2 ([4]) $P_2 \cup P_{n-2} \succ P_4 \cup P_{n-4} \succ \cdots \succ P_3 \cup P_{n-3} > P_1 \cup P_{n-1}$.

In [13] it was demonstrated that C_n attains the maximal matching energy in unicyclic graphs. The following lemma determined the unicyclic graph having the second-maximal matching energy:

Lemma 2.3 *Let G be a unicyclic graph of order n, other than C_n . Then $ME(G) \leq ME(P_n^4)$, the equality holds if and only if $G \cong P_n^4$ or P_n^{n-2} .*

Proof. Observe that the girth of a unicyclic graph G is no more than $n - 1$ which means that G contains at least one pendent vertex. (Since, C_n is not contained in unicyclic graphs on condition.) In view of quasi-order, it is sufficient to show $m(G, k) \leq m(P_n^4, k)$ for $1 \leq k \leq \lfloor n/2 \rfloor$. By means of Proposition 2.1, we have

$$m(P_n^4, k) = m(P_n, k) + m(P_2 \cup P_{n-4}, k - 1) \ . \tag{2.3}$$

For a unicyclic graph G, through choosing a proper edge $uv = e$, we get

$$\begin{aligned} m(G, k) &= m(G - e, k) + m(G - u - v, k - 1) \\ &\leq m(P_n, k) + m(P_2 \cup P_{n-4}, k - 1) \ . \end{aligned} \tag{2.4}$$

The equality holds in Ineq. (2.4) if and only if $m(G - e, k) = m(P_n, k)$ and $m(G - u - v, k - 1) = m(P_2 \cup P_{n-4}, k - 1)$, which means that $G \cong P_n^i$, $(i = 4 \, or \, n - 2)$. ■

We next introduce an important result, which will be used in the proof of Theorem 3.3.

Lemma 2.4 $P_2 \cup P_{n-2}^4 \succ P_i \cup P_{n-i}^{i+2}$, *where* $2i + 2 < n$ $(i.e., P_{n-i}^{i+2} \ncong C_{n-i})$.

Proof. In terms of the quasi-order, it is sufficient to show $m(P_2 \cup P_{n-2}^4, k) \geq m(P_i \cup P_{n-i}^{i+2}, k)$ for all $1 \leq k \leq \lfloor n/2 \rfloor$. In view of Eq. (2.1), we have

$$\begin{aligned} m(P_i \cup P_{n-i}^{i+2}, k) &= m(P_i \cup P_{n-i}, k) + m(P_i \cup P_{n-2i-2} \cup P_i, k-1) \\ &\leq m(P_i \cup P_{n-i}, k) + m(P_2 \cup P_{n-i-4} \cup P_i, k-1) \\ &< m(P_2 \cup P_{n-2}, k) + m(P_2 \cup P_{n-6} \cup P_2, k-1) = m(P_2 \cup P_{n-2}^4, k) \ . \end{aligned}$$

By Lemma 2.2 , the proof is thus complete. ∎

3 Extremal matching energy in bicyclic graphs

We first discuss the graph possessing minimal matching energy in $\mathscr{B}_n$.

Theorem 3.1 *Let $G \in \mathscr{B}_n$ with $n \geq 4$. Then $ME(G) \geq ME(S_n^*)$ with equality if and only if $G \cong S_n^*$.*

Proof. Note that $m(S_n^*, 1) = n+1$, $m(S_n^*, 2) = 2(n-3)$, $m(S_n^*, k) = 0$ for $k \geq 3$. For any graph $G \ncong S_n^*$, $m(G, 1) = m(S_n^*, 1)$. By the quasi-order, it is sufficient to show that $m(G, 2) > m(S_n^*, 2)$. We will prove this by induction on n. When $n = 4$, this case is trivial. When $n = 5$, there are only five distinct graphs and it is easy to check the correctness of the conclusion. We now assume that the result holds on $|S_n^*| = |G| < n$. Suppose that $|G| = n$. Two cases should be discussed.

Case 1. G contains at least one pendent vertex.

Let u be a pendent vertex of G which just connects vertex v and u' be a pendent vertex of S_n^*. According to Eq. (2.2), we have

$$\begin{aligned} m(G, 2) &= m(G-u, 2) + m(G-u-v, 1) \\ m(S_n^*, 2) &= m(S_n^* - u', 2) + m(P_3, 1) \ . \end{aligned}$$

Since $G-u$ is a bicyclic graph with $|G-u| < n$, by the induction hypothesis, $m(G-u, 2) > m(S_{n-1}^*, 2)$. Moreover, we should consider the resulted graph $G-u-v$ with order not less than 4.

When v is not a cut vertex of the graph $G-u$, then $G-u-v$ is a connected graph, and contains P_3 as its proper subgraph. So $m(G-u-v, 1) \geq 3 > m(P_3, 1)$.

When v is a cut vertex of graph $G-u$, then $G-u-v$ consists of some connected components. Note that it includes at least one non-trivial component (trivial component is referred to the graph with order 1.). Otherwise we can deduce that G is isomorphic to a tree with diameter two which contradicts to the fact that G is bicyclic. If $G-u-v$ contains only one non-trivial component, set H_1. Then H_1 includes cycle and with $|H_1| \geq 3$. Hence, $m(G-u-v,1) \geq m(H_1,1) \geq 3 > m(P_3,1)$. If $G-u-v$ possesses at least H_2 and H_3 as its non-trivial components, then the their sizes are not less than one. Thus, $m(G-u-v,1) \geq m(H_2 \cup H_3, 1) \geq m(P_3,1)$.

Therefore, $m(G,2) > m(S_n^*,2)$.

Case 2. G doesn't contain any pendent vertex.

In terms of Eq. (2.1), selecting an edge $e = uv$ in G and an edge $e_1 = u'v'$ with $d(u') = 3$ and $d(v') = 2$, we have

$$m(G,2) = m(G-e,2) + m(G-u-v,1)$$
$$m(S_n^*,2) = m(S_n^* - e_1, 2) + m(S_{n-2},1) \ .$$

Note that $S_n^* - e_1 \cong S_n^+$ and $G-e$ is a unicyclic graph. Combining a unicyclic result in [13], we deduce that $m(G-e,2) \geq m(S_n^* - e_1, 2)$. In addition, it is not difficult to find that $m(G-u-v,1) > m(G-u-v-e_2,1) \geq m(S_{n-2},1)$, where $G-u-v-e_2$ is an acyclic connected spanning subgraph of $G-u-v$. Hence, $m(G,2) > m(S_n^*,2)$.

Therefore, the proof is complete. ■

In the following, we consider the maximal matching energy in bicyclic graphs.

Theorem 3.2 *If $G_0 \in \mathscr{B}_n^1$, then $ME(G_0) \leq ME(C_n(3,1,n-3))$ for $n \geq 6$.*

Proof. According to Proposition 2.1, by choosing an $e = uv$ edge with $d(u) = 3$ and e in the path P_{3+1}, we have that

$$m(C_n(3,1,n-3),k) = m(P_n^{n-2},k) + m(P_{n-2},k-1) \ .$$

Note that every graph G_0 in $\mathscr{B}_n^1$ has a brace as $C_s(\ell,r,t)$. We now discuss the value of r in the brace $C_s(\ell,r,t)$, so the following two cases should be considered.

Case 1. $r \geq 2$. (It means that $|C_{\ell+r}|, |C_{r+t}| \geq 4$.)

Case 1.1 $|C_s(\ell,r,t)| = n$

In this case, graph $G_0(\cong C_n(\ell,r,t))$ doesn't contain any pendent vertex. We now choose an edge $e = uv$ on P_{r+1} with $d(u) = 3$. By Proposition 2.1, we get

$$\begin{aligned} m(C_n(\ell,r,t),k) &= m(C_n(\ell,r,t)-uv,k) + m(C_n(\ell,r,t)-u-v,k-1) \\ &\leq m(P_n^{n-2},k) + m(P_{n-2},k-1) = m(C_n(3,1,n-3),k) \ . \end{aligned}$$

In view of the quasi-order, the result holds.

Case 1.2 $|C_s(\ell,r,t)| < n$.

In this case, graph G_0 has at least one pendent vertex. According to the quasi-order, we chose an edge $e = uv$ with $d(u) = 3$ in the brace $C_s(\ell, r, t)$ and v in $P_{\ell+1}$ such that $G_0 - u - v$ is a forest. Then by Lemma 2.4,

$$\begin{aligned} m(G_0, k) &= m(G_0 - uv, k) + m(G_0 - u - v, k - 1) \\ &\le m(P_n^{n-2}, k) + m(P_{n-2}, k - 1) = m(C_n(3, 1, n - 3), k) \ . \end{aligned}$$

In the above inequalities, there exists at least a inequality which is strict for $G_0 \ncong C_n(3, 1, n - 3)$.

Case 2. $r = 1$.

If G_0 does not have any pendent vertex, then $G_0 \cong C_n(\ell, 1, t)$. We choose an edge $e' = u'v'$ such that $d(u') = 3$ and e' belongs to the path $P_{\ell+1}$. If G_0 has at least one pendent vertex, then the size of the brace $C_s(\ell, 1, t)$ is less than n. We choose an edge $e_1 = u_1v_1$ with $d(u_1) = 3$ in brace $C_s(\ell, 1, t)$ and e' in the path $P_{\ell+1}$. Using the analogous method on case 1, it is not difficult to show that $G_0 \prec C_n(3, 1, n-3)$. So the result holds.

This completes the proof. ■

Theorem 3.3 *Let G be a graph in $\mathscr{B}_2$ with $d_G \ge 2$. Then $ME(G) \le ME(P_n^{4,4})$. Equality holds if and only if $G \cong P_n^{4,4}$.*

Proof. Notice that $G \in \mathscr{B}_2$ means that G has a subgraph of the form $P_s^{\ell,r}$. Two cases will be discussed.

Case 1. G contains at least one pendent vertex. According to the definition of $P_s^{\ell,r}$, we denote the path connecting the two cycles by T. By Eq. (2.1), we choose an edge $e = uv$ with vertex u being the end-vertex of the path T and v be a vertex in a cycle of G. By this way, $G - u - v$ is an union of a forest and an unicyclic graph. Then by Lemmas 2.4 and 2.3,

$$\begin{aligned} m(G, k) &= m(G - uv, k) + m(G - u - v, k - 1) \\ &\le m(P_n^4, k) + m(P_2 \cup P_{n-4}^4, k - 1) = m(P_n^{4,4}, k) \ . \end{aligned}$$

Case 2. G does not have any pendent vertex, which means that $G \cong P_n^{\ell,r}$.

By Eq. (2.1), choosing an edgee $= uv$ such that $d(u) = 3$ and v belongs to the cycle C_ℓ, we obtain

$$\begin{aligned} m(G, k) &= m(G - uv, k) + m(G - u - v) \\ &= m(P_n^r, k) + m(P_{\ell-2} \cup P_{n-\ell}^r, k - 1) \\ &\le m(P_n^4, k) + m(P_2 \cup P_{n-4}^4, k - 1) = m(P_n^{4,4}, k) \end{aligned}$$

where Lemmas 2.3 and 2.4 have been used. Hence, the conclusion holds. ■

Theorem 3.4 *For all graphs in $\mathscr{B}_2$ with $d = 0, 1$, the graph $P_n^{4,n-4}$ has the maximal matching energy.*

Proof. Before giving a whole proof of the above assertion, we will verify the following claim.

Claim 1. $P_2 \cup C_{n-4} \succ P_i \cup C_{n-i-2}$.

Proof. In terms of Proposition 2.1, we obtain

$$m(P_2 \cup C_{n-4}, k) = m(P_2 \cup P_{n-4}, k) + m(P_2 \cup P_{n-6}, k-1)$$
$$m(P_i \cup C_{n-i-2}, k) = m(P_i \cup P_{n-i-2}, k) + m(P_i \cup P_{n-i-4}, k-1) \ .$$

By Lemma 2.2,

$$m(P_2 \cup P_{n-4}, k) \succeq m(P_i \cup P_{n-i-2}, k)$$
$$m(P_2 \cup P_{n-6}, k-1) \succeq m(P_i \cup P_{n-i-4}, k-1) \ .$$

If all equalities holds in above relations, then $i = 2$ or $i = n-4$ with Lemma 2.2. According to the condition, i just equals to 2. In other words, equalities holds if and only if $P_i \cup C_{n-i-2} \cong P_2 \cup C_{n-4}$. ■

Using the same method in the proof of Theorem 3.3, together with Claim 1, we can verify that $ME(G_0) \leq ME(P_n^{4,n-4})$ for $G_0 \in \mathscr{B}_2$, and that equality holds if and only if $G_0 \cong P_n^{4,n-4}$. ■

We now introduce two important conclusions, and determine the graph possessing maximal matching energy in $\mathscr{B}_n$.

Theorem 3.5 $ME(C_n(3,1,n-3)) < ME(P_n^{4,n-4})$ *for* $n \geq 10$ *and* $n = 8$*, exceptionally* $ME(C_n(3,1,n-3)) < ME(P_n^{4,n-4})$ *for* $n = 9$*.*

Proof. For $n \geq 10$ and $n = 8$, by choosing an edge $uv = e$ with $d(u)$ (or $d(v)) = 3$, we get

$$\begin{aligned}
m(C_n(3,1,n-3), k) &= m(P_n^4, k) + m(P_{n-2}, k-1) \\
&= m(P_n^4, k) + m(P_4 \cup P_{n-6}, k-1) + m(P_3 \cup P_{n-7}, k-2) \\
&\leq m(P_n^4, k) + m(P_4 \cup P_{n-6}, k-1) + m(P_2 \cup P_{n-6}, k-2) \\
&= m(P_n^4, k) + m(C_4 \cup P_{n-6}, k-1) = m(P_n^{4,n-4}, k)
\end{aligned}$$

from Lemma 2.2. Note that at least one of these inequalities is strict for some k.

In fact, the two numbers are equal on the two side of the third inequality for $n = 9$. Since $m(P_3 \cup P_{n-7}, k-2) = m(P_2 \cup P_{n-6}, k-2)$ with $n = 9$.

Therefore, the proof is complete. ■

Theorem 3.6 *$ME(P_n^{4,4}) < ME(P_n^{4,n-4})$, where $n \geq 9$.*

Proof. For exhibiting the proceeding of the proof, we firstly show a claim.

Claim 2. $m(2P_1 \cup P_{n-6}, k) + m(P_2 \cup P_{n-8}, k-1) \geq m(2P_2 \cup P_{n-8}, k)$.

Proof. In view of Proposition 2.1, one can deduce that

$$\begin{aligned} & m(2P_1 \cup P_{n-6}, k) + m(P_2 \cup P_{n-8}, k-1) \\ = \; & m(2P_1 \cup P_2 \cup P_{n-8}, k) + m(3P_1 \cup P_{n-9}, k-1) \\ + \; & m(P_2 \cup P_{n-8}, k-1) \\ \geq \; & m(2P_1 \cup P_2 \cup P_{n-8}, k) + m(P_2 \cup P_{n-8}, k-1) = m(2P_2 \cup P_{n-8}, k) \end{aligned}$$

so that the Claim holds. ■

We now go back to the proceeding of the proof. By means of Proposition 2.1, by choosing an edge $e = uv$ with u be an end-vertex of T and v be a vertex in C_{n-4}, we have

$$\begin{aligned} m(P_n^{4,n-4}, k) &= m(P_n^4, k) + m(C_4 \cup P_{n-6}, k-1) \\ &= m(P_n^4, k) + m(P_4 \cup P_{n-6}, k-1) + m(P_2 \cup P_{n-6}, k-2) \\ &= m(P_n^4, k) + m(2P_2 \cup P_{n-6}, k-1) + m(2P_1 \cup P_{n-6}, k-2) \\ &+ m(P_2 \cup P_{n-6}, k-2) \\ &= m(P_n^4, k) + m(2P_2 \cup P_{n-6}, k-1) + m(2P_1 \cup P_{n-6}, k-2) \\ &+ m(P_2 \cup P_1 \cup P_{n-7}, k-2) + m(P_2 \cup P_{n-8}, k-3) \\ \text{(by Claim 2)} &\geq m(P_n^4, k) + m(2P_2 \cup P_{n-6}, k-1) + m(2P_2 \cup P_{n-8}, k-2) \\ &+ m(P_2 \cup P_1 \cup P_{n-7}, k-2) \\ &= m(P_n^4, k) + m(P_2 \cup P_{n-4}, k-1) + m(2P_2 \cup P_{n-8}, k-2) \\ &= m(P_n^4, k) + m(P_2 \cup P_{n-4}^4, k-1) = m(P_n^{4,4}, k) \; . \end{aligned}$$

Therefore, the proof is complete. ■

Combining Theorems 3.1, 3.5, and 3.6, we deduce the conclusion of Theorem 1.3.

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