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Graphs with Extremal Matching Energies and Prescribed Parameters *

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Abstract

Gutman and Wagner [I. Gutman, S. Wagner, The matching energy of a graph, Discrete Appl. Math. 160 (2012) 2177-2187] defined the matching energy of a graph and gave some properties of the matching energy, especially in characterizing the extremal graphs among some classes of graphs. Further, the graphs with maximum matching energy and given connectivity (resp. chromatic number) were characterized by Li and Yan. In this paper, the unicyclic graphs with fixed girth and the graphs with given clique number are characterized in terms of maximum and minimum matching energy.

1 Introduction

In 2012, Gutman and Wagner [5] defined the matching energy of a graph G, denoted by $ME(G)$, as

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

As pointed out in [5], the matching energy is a quantity of relevance for chemical applications, which may be supported by the simple relation $\mathrm{TRE}(G) = \mathrm{E}(G) - \mathrm{ME}(G)$,

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where TRE(G) and E(G) stand for the topological resonance energy and energy of G, respectively. It is also noticed that if the graph G is a forest, its matching energy coincides with its energy. The energy of a graph was also introduced by the same scholar Gutman in [6] and has been studied extensively (see [6, 8, 11]).

All graphs under discussion are finite, undirected and simple. A *matching* in a graph is a set of pairwise nonadjacent 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 $m_0(G) = 1$. Matching theory has been an active and can be found applicable in numerous fields [13]. One of those concerning matching is the well-known Hosoya index [7], defined as the total number of matchings, including the empty edges set, of a graph. Another is the matching polynomial of a graph G of order n, defined as

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

where the convention that $m_k(G) = 0$ for $k < 0$ or $k > n/2$ is adopted. For any graph G, all the zeros of $\alpha(G,x)$ are real-valued and the theory of matching polynomial is well elaborated in [1, 2, 4, 3]. Recall the following result in [5].

Theorem 1 ([5]). *Let G be a simple graph, and let $\mu_1, \mu_2, \ldots, \mu_n$ be the zeros of its matching polynomial. Then*

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

This makes us believe that the matching energy of a graph may have an important role to play in studying the matching of a graph.

The integral on the right hand side of Eq.(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

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

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 $G \succeq H \Longrightarrow ME(G) \geq ME(H)$ and $G \succ H \Longrightarrow ME(G) > ME(H)$. From this fact, one can readily deduce the extremal graphs for matching energy.

Given a graph G and an edge uv of G, we denote by $G - uv$ (resp. $G - v$) the graph obtained from G by deleting the edge uv (resp. the vertex v and edges incident to it).

Lemma 1 ([1])**.** *If u, v are adjacent vertices of G, then*

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

for all nonnegative integers k.

From the lemma above, it follows that $m_k(G)$ can only increase when edges are added to a graph and the following observation has been obtained in [5].

Theorem 2 ([5])**.** *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*

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

Consequently, a series of results concerning the extremal graphs of matching energy can be obtained by the nice property of matching energy. Denote by K_n and S_n the complete graph and star on n vertices, respectively.

Corollary 1 ([5])**.** *Among all graph on n vertices, the empty graph E_n without edges and the complete graph K_n have, respectively, minimum and maximum matching energy.*

Corollary 2 ([5])**.** *The connected graph on n vertices having minimum matching energy is the star S_n.*

Denote by $\mathcal{U}_n$ the set of all connected unicyclic graphs on n vertices. Let C_n be the n-vertex cycle, and let S_n^+ be the graph obtained by adding a new edge to the star S_n.

Theorem 3 ([5])**.** *If $G \in \mathcal{U}_n$, then*

$$ME(S_n^+) \leq ME(G) \leq ME(C_n)$$

with equality if and only if $G \cong S_n^+$ and $G \cong C_n$, respectively.

Cutman and Wagner also pointed out the following result.

Lemma 2 ([5]). *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).*

After then, Ji, Li and Shi [9] characterized the graphs with the extremal matching energy among all bicyclic graphs. Li and Yan [12] characterized the connected graph with the given connectivity (resp. chromatic number) which has maximum matching energy. Particularly, the following result concerning chromatic number is listed which will be used in the sequel. Recall that *Turán graph* $T_{\chi,n}$ is complete χ-partite graph on n vertices in which all parts are as equal in size as possible. The *chromatic number* $\chi(G)$ of a graph G is the minimum number of colors such that G can be colored with these colors in such a way that no two adjacent vertices have the same color.

Lemma 3 ([12]). *Let G be a connected graph of order n with chromatic number χ. Then*

$$ME(G) \leq ME(T_{\chi,n}).$$

The equality holds if and only if $G \cong K_{\underbrace{r,\ldots,r}_{\chi-s},\underbrace{r+1,\ldots,r+1}_{s}}$, where r and s are integers with $n = r\chi + s$ and $0 \leq s \leq \chi$.

In this paper, we characterize the unicyclic graphs of order n with fixed girth and extremal (i.e., maximum and minimum) matching energy. Meanwhile, the extremal graphs among all connected graphs with given order and clique number are characterized.

2 Main results

First recall some notations and a result in [10]. Denote by $\mathcal{U}_{g,n}$ the set of unicyclic graphs with n vertices and a cycle of length g. The sun graph, denoted by $C_g(P_{r_1+1}, \ldots, P_{r_g+1})$, is one obtained from the cycle $C_g = v_1v_2\cdots v_gv_1$ by identifying one pendant vertex of path P_{r_i+1} with vertex v_i for $i = 1, \ldots, g$. Note that $C_g(P_{n-g+1}, P_1, \ldots, P_1)$ is also called lollipop graph and denoted by $E_{g,n}$, as shown in Figure 1. Similarly, $C_g(S_{r_1+1}, \ldots, S_{r_g+1})$ stands for the uncyclic graph of the cycle $C_g = v_1v_2\cdots v_gv_1$ together with r_i pendant edges attached at vertex v_i for $i = 1, \ldots, g$, where $r_1, \ldots, r_g$ are nonnegative integers. Also, in particular, $C_g(S_{n-g+1}, S_1, \ldots, S_1)$ is simply denoted by $C_g(S_{n-g+1})$, as given in Figure 1.

(i) $C_g(S_{n-g+1})$ (ii) $E_{g,n}$

Fig. 1 The graphs $C_g(S_{n-g+1})$ and $E_{g,n}$.

Theorem 4 ([10])**.** *Let n, g be any positive integers, $n > g \geq 3$. For any $G \in \mathcal{U}_{g,n}$, $m_k(E_{g,n}) \geq m_k(G)$ for all positive integers k.*

From Theorem 4, it follows immediately that $E_{g,n} \succeq G$ for any $G \in \mathcal{U}_{g,n}$, and so $ME(E_{g,n}) \geq ME(G)$. To show the uniqueness of $E_{g,n}$ as maximum graph, it suffices to prove that $E_{g,n} \succ G$ for any $G \in \mathcal{U}_{g,n} \backslash \{E_{g,n}\}$, which is solved in the following.

Theorem 5. *Let n, g be positive integers, $n > g \geq 3$. For any connected graph $G \in \mathcal{U}_{g,n}$, we have*

$$ME(E_{g,n}) \geq ME(G)$$

with equality if and only if $G \cong E_{g,n}$.

Proof. From Theorem 4, it suffices to show that for any $G \in \mathcal{U}_{g,n} \backslash \{E_{g,n}\}$, $m_k(E_{g,n}) > m_k(G)$ for some k. Now we show that this holds at least for the case of $k = 2$.

Any graph $G \in \mathcal{U}_{g,n}$ can be viewed as obtained from a cycle C_g together with some trees rooted on the cycle vertices. By Lemma 2, when any rooted tree is replaced by a path with one end at the cycle vertex, the matching energy increases unless the rooted tree is already such a path. After replacing all rooted trees of G with paths, the resulting graph is of the form sun graph. Therefore, to prove that $ME(E_{g,n}) > ME(G)$ for any $G \in \mathcal{U}_{g,n} \backslash \{E_{g,n}\}$, it suffices to prove that the matching energy of all sun graphs with girth g and order n which is not a lollipop graph is always less than that of $E_{g,n}$.

Next we shall show that for any sun graph $C_g(P_{r_1+1}, P_{r_2+1}, \ldots, P_{r_g+1})$ which is not a lollipop graph, $m_2(E_{g,n}) > m_2(C_g(P_{r_1+1}, P_{r_2+1}, \ldots, P_{r_g+1}))$. Let $t = |\{i | r_i > 0\}|$. Because

$C_g(P_{r_1+1}, P_{r_2+1}, \ldots, P_{r_g+1})$ is not a lollipop graph, $t \geq 2$ and say $r_1, r_2 > 0$, without loss of generality. Recall a formula used in [5], that is

$$m_2(G) = \binom{m}{2} - \sum_{i=1}^{n} \binom{d_i}{2},$$

where m denotes the number of edges in G and d_i the degree of the i-th vertex for $i = 1, \ldots, n$. We have

$$\begin{aligned} m_2(C_g(P_{r_1+r_2+1}, P_1, P_{r_3+1}, \ldots, P_{r_g+1})) - m_2(C_g(P_{r_1+1}, P_{r_2+1}, \ldots, P_{r_g+1})) \\ = - \left[\binom{2}{2} + \binom{2}{2}\right] + \left[\binom{3}{2} + \binom{1}{2}\right] \\ = 1. \end{aligned}$$

Continuing the process above, we ultimately come to

$$m_2(E_{g,n}) - m_2(C_g(P_{r_1+1}, P_{r_2+1}, \ldots, P_{r_g+1})) = t - 1.$$

Since $t \geq 2$, $m_2(E_{g,n}) - m_2(C_g(P_{r_1+1}, P_{r_2+1}, \ldots, P_{r_g+1})) > 0$ and so we are done. ■

Theorem 6. *Let n, g be positive integers, $n > g \geq 3$. For any graph $G \in \mathcal{U}_{g,n}$, we have*

$$ME(C_g(S_{n-g+1})) \leq ME(G)$$

with equality if and only if $G \cong C_g(S_{n-g+1})$.

Proof. By Lemma 2, for any graph $G \in \mathcal{U}_{g,n}$, its matching energy decreases when any tree rooted at cycle vertex is replaced with a star centered at the cycle vertex. Thus it suffices to prove that the assertion holds for any such graph G of the form $C_g(S_{r_1+1}, \ldots, S_{r_g+1})$.

Let $G = C_g(S_{r_1+1}, \ldots, S_{r_g+1})$, with the unique cycle $C_g = u_1 u_2 \cdots u_g u_1$ and r_i pendant edges attached at vertex u_i for $i = 1, \ldots, g$. We proceed by induction on t, where $t = \sum_{i=1}^{g} r_i$, i.e., the number of pendant edges of G. Clearly $t \geq 1$ as $n > g$. If $t = 1$, then $G = C_{n-1}(S_2)$ and there is nothing to prove. Now suppose that $t > 1$ and the result is valid for the graphs with less than t pendant edges. Without loss of generality, suppose that $r_1 > 0$ and $u_1 v_1$ is a pendent edge at the vertex u_1 lying on the cycle of G. By Lemma 1, we have

$$\begin{aligned} m_k(G) =& m_k(G - u_1 v_1) + m_{k-1}(G - u_1 - v_1) \\ =& m_k(C_g(S_{r_1}, S_{r_2+1}, \ldots, S_{r_g+1})) \\ &+ m_{k-1}(C_g(S_1, S_{r_2+1}, \ldots, S_{r_g+1}) - u_1), \end{aligned}$$

and

$$m_k(C_g(S_{n-g+1})) = m_k(C_g(S_{n-g})) + m_{k-1}(P_{g-1}) \; .$$

Since $C_g(S_{r_1}, S_{r_2+1}, \ldots, S_{r_g+1})$ has less than t pendant edges, by the induction hypothesis,

$$m_k(C_g(S_{r_1}, S_{r_2+1}, \ldots, S_{r_g+1})) \geq m_k(C_g(S_{n-g})).$$

Meanwhile, note that P_{g-1} is a proper subgraph of graph $C_g(S_1, S_{r_2+1}, \ldots, S_{r_g+1}) - u_1$, so the number of k-matchings of the former is always not more than that of the latter. In particular, $m_1(P_{g-1}) < m_1(C_g(S_1, S_{r_2+1}, \ldots, S_{r_g+1}) - u_1)$. So we conclude that

$$m_k(C_g(S_{r_1+1}, S_{r_2+1}, \ldots, S_{r_g+1})) \geq m_k(C_g(S_{n-g+1})),$$

holds for all k and the inequality is strict at least for $k = 2$. So $C_g(S_{r_1+1}, S_{r_2+1}, \ldots, S_{r_g+1}) \succ C_g(S_{n-g+1})$.

We can now conclude that $G \succ C_g(S_{n-g+1})$ for any graph $G \in \mathcal{U}_{g,n} \setminus \{C_g(S_{n-g+1})\}$. The proof of the theorem is complete. ■

A *complete graph* is a simple graph in which any two vertices are adjacent. A complete subgraph of G is called a *clique* of G and that the maximum size of a clique of a graph G is called the *clique number* of G. Next we shall investigate the extremal graphs with fixed clique number in terms of matching energy. Among all graphs with clique number l and order n, it is easily to verify that the graph $K_l \cup E_{n-l}$, where E_{n-l} is the empty graph on $n - l$ vertices, uniquely attains minimum matching energy. So we only need to consider the connected ones.

We denote by $\omega_{n,l}$ the set of connected graphs with clique number l and n vertices. Denote by $K_l(S_{r_1+1}, S_{r_2+1}, \ldots, S_{r_l+1})$ the connected graphs which consist of the clique K_l with $V(K_l) = \{v_1, v_2, \ldots, v_l\}$ and r_i pendant edges attached at vertex v_i for $i = 1, \ldots, l$, where $r_1, \ldots, r_g$ are nonnegative integers. $K_l(S_{n-l+1}, S_1, \ldots, S_1)$ is simply written as $K_l(S_{n-l+1})$, and $K_5(S_{n-4})$ is, for example, given in Figure 2.

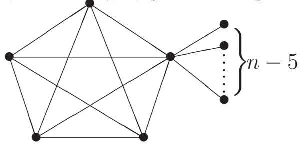

Fig. 2 The graph $K_5(S_{n-4})$.

Theorem 7. *For any graph $G \in \omega_{n,l}$, we have*

$$ME(G) \geq ME(K_l(S_{n-l+1}))$$

with equality if and only if $G \cong K_l(S_{n-l+1})$.

Proof. Any graph $G \in \omega_{n,l}$ has an induced subgraph K_l and let the vertices of the clique be labelled as $v_1, v_2, \ldots, v_l$. Suppose that G has the minimum matching energy in $\omega_{n,l}$. By Theorem 2, G must have as the least number of edges in $\omega_{n,l}$ as possible. Then G can be thought of as obtained from K_l by attaching some trees rooted at some vertices of K_l.

From Lemma 2, replacing any such rooted tree with a star centered at the vertex of the clique decreases its matching energy. Therefore we can assume that G is already of the form $K_l(S_{r_1+1}, S_{r_2+1}, \ldots, S_{r_l+1})$. Next we shall show that for any k, $m_k(K_l(S_{r_1+1}, S_{r_2+1}, \ldots, S_{r_l+1})) \geq m_k(K_l(S_{n-l+1}))$. We proceed by induction on t, where $t = \sum_{i=1}^{l} r_i$, i.e., the number of pendant edges of G. If $t = 1$, there is nothing to prove. So suppose that $t > 1$ and the result is valid with less than t pendant edges. Without loss of generality, suppose that $r_1 > 0$ and v_1u_1 is a pendant edge at the vertex v_1 lying on the clique of G. By Lemma 1, we have

$$\begin{aligned} & m_k(K_l(S_{r_1+1}, S_{r_2+1}, \ldots, S_{r_l+1})) \\ &\quad = m_k(K_l(S_{r_1+1}, S_{r_2+1}, \ldots, S_{r_l+1}) - v_1u_1) \\ &\qquad + m_{k-1}(K_l(S_{r_1+1}, S_{r_2+1}, \ldots, S_{r_l+1}) - v_1 - u_1) \\ &\quad = m_k(K_l(S_{r_1}, S_{r_2+1}, \ldots, S_{r_l+1})) + m_{k-1}(K_{l-1}(S_{r_2+1}, \ldots, S_{r_l+1})), \end{aligned}$$

and

$$m_k(K_l(S_{n-l+1})) = m_k(K_l(S_{n-l})) + m_{k-1}(K_{l-1}).$$

Since $K_l(S_{r_1}, S_{r_2+1}, \ldots, S_{r_l+1})$ has less than t pendant edges, by the induction hypothesis,

$$m_k(K_l(S_{r_1}, S_{r_2+1}, \ldots, S_{r_l+1})) \geq m_k(K_l(S_{n-l})).$$

In the meantime, K_{l-1} is a proper subgraph of $K_{l-1}(S_{r_2+1}, \ldots, S_{r_l+1})$, which implies that for all k the number of k-matchings of the former is always not more than that of the latter. Particularly, $m_1(K_{l-1}(S_{r_2+1}, \ldots, S_{r_l+1})) > m_1(K_{l-1})$. This follows that

$m_k(K_l(S_{r_1+1}, S_{r_2+1}, \ldots, S_{r_l+1})) \geq m_k(K_l(S_{n-l+1}))$ for all k and the inequality is strict for $k = 2$. Consequently, $ME(K_l(S_{n-l+1})) < ME(G)$ provided $G \in \omega_{n,l} \setminus \{K_l(S_{n-l+1})\}$. ■

Theorem 8. *For any graph $G \in \omega_{n,l}$, we have*

$$ME(G) \leq ME(T_{l,n}),$$

with equality if and only if $G \cong T_{l,n}$.

Proof. Suppose that $G \in \omega_{n,l}$ has the maximum matching energy. Note that first G has K_l as its subgraph and suppose its vertices are labelled as $v_1, v_2, \ldots, v_l$. Initially, let $V_i := \{v_i\}$, for $i = 1, \ldots, l$. In order to obtain graph G from K_l, we need to add the remaining vertices to subgraph K_l and denote these vertices by $v'_1, v'_2, \ldots, v'_{n-l}$.

First, add the vertex v'_1 to the subgraph K_l and the resultant graph is denoted by G_1. Considering the clique number of the resultant graph in each step cannot exceed l, the vertex v'_1 is adjacent to at most $l-1$ vertices on the clique K_l. On the other hand, v'_1 must be adjacent to exactly $l-1$ vertices on the clique K_l, because G has the maximum matching energy in $\omega_{n,l}$ and so G (hence G_1) has as many edges as possible. Thus v'_1 is not adjacent to exactly one vertex, say v_1. Then set $V_1 := \{v_1, v'_1\}$ in G_1, while other V_i's remain unchanged.

Now add vertex v'_2 to G_1 and the resultant graph is denoted by G_2. If there is always a vertex in each part V_i $(1 \leq i \leq l)$ which is adjacent to v'_2, then the clique number of the resultant graph would surpass l, a contradiction with that $G \in \omega_{n,l}$. Thus v'_2 can be adjacent to at most $l-1$ parts V_i. Meanwhile, note that v'_2 can be adjacent to all vertices in these $l-1$ parts, without causing its clique number to surpass l. Since G_2 has as many edges as possible, v'_2 is not adjacent to precisely one part, say V_2. Set $V_2 := V_2 \cup \{v'_2\}$.

Continuing the process above, ultimately we come to the resultant graph G_{n-l}, which is already G. Obviously G obtained in this way must be complete l-partite graph on n vertices. So $\chi(G) = l$.

Based on $\chi(G) = l$ and Lemma 3, we have $ME(G) \leq T_{l,n}$. Note that $T_{l,n} \in \omega_{n,l}$ also, then the theorem follows immediately. ■

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