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Bipartite Graphs with Extremal Matching Energies with Given Matching Number

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Abstract

Let G be a simple graph with 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 $\mu_i (i = 1, 2, \ldots, n)$, which was proposed by Gutman and Wagner. A maximum matching is one which covers as many vertices as possible. The number of edges in a maximum matching of a graph G is called the matching number of G and denoted by $\alpha'(G)$. Let $\mathcal{B}(n, \beta)$ and $\mathcal{UB}(n, \beta)$ be the set of connected bipartite graphs and connected bipartite unicyclic graphs with order n and matching number β, respectively. In this paper, we characterize graphs with the first three largest matching energies in $\mathcal{B}(n, \beta)$. Also we determine the extremal graph with minimal and the second minimal matching energy among graphs in $\mathcal{B}(n, \beta)$, respectively. Furthermore, we determine the extremal graph from $\mathcal{UB}(n, \beta)$ minimizing the matching energy.

1 Introduction

In this paper, all graphs under our consideration are finite, connected, undirected and simple. Let G be a graph with n vertices and $A(G)$ be its adjacency matrix. The *characteristic polynomial* of G, denoted by $\phi(G)$, is defined as

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

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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 G, denoted by $E(G)$, is defined as

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

The concept of graph energy was proposed by Gutman in [13] and now is well-studied. For details, we refer the book on graph energy [26] and some new recent references [20,21,27].

Let G be a graph with n vertices and m edges. A *matching* in G is a set of pairwise nonadjacent edges and its size is the number of edges in it. A matching M with size k is called a *k-matching*. Denote by $m(G,k)$ the number of k-matchings of G. In particular, $m(G,1) = m$ and $m(G,k) = 0$ for $k > \lfloor \frac{n}{2} \rfloor$ or $k < 0$. In addition, define $m(G,0) = 1$. Then the *matching polynomial* of the graph G is defined as

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

For more details of the results on the matching polynomial of the graph, please refer to [11, 12, 14].

In [18], Gutman and Wagner firstly proposed the concept of matching energy. They defined the *matching energy* of a graph G as follows:

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

where $\mu_i (i = 1, 2, \ldots, n)$ are the roots of $\alpha(G,\mu) = 0$. Besides, Gutman and Wagner also gave the following equivalent definition of matching energy.

Definition 1.1 **([18])** *Let G be a simple graph, and let $m(G,k)$ be the number of its k-matchings, $k = 0, 1, 2, \ldots$. The matching energy of G is*

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

Eq. (1) is called the *Coulson integral formula* of matching energy. Obviously, by the monotonicity of the logarithm function, Eq. (1) implies that the matching energy of a graph G is a monotonically increasing function of any $m(G,k)$. Then we can define a *quasi-order* "$\succeq$" as follows: for two graphs G_1 and G_2,

$$G_1 \succeq G_2 \Longleftrightarrow m(G_1,k) \geq m(G_2,k) \ for \ all \ k. \tag{2}$$

If $G_1 \succeq G_2$ and there exists some k such that $m(G_1,k) > m(G_2,k)$, then we write $G_1 \succ G_2$. According to Eq.(1) and Eq.(2), we get the following results directly

$$G_1 \succeq G_2 \Longrightarrow ME(G_1) \geq ME(G_2) \tag{3}$$

$$G_1 \succ G_2 \Longrightarrow ME(G_1) > ME(G_2) \tag{4}$$

In [18], Gutman and Wagner 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 [17].

The matching energy of a graph is widely studied in recent years. In [18], Gutman and Wagner gave some elementary results on the matching energy and obtained the unicyclic graphs with minimal and maximal matching energy. For the bicyclic graphs, Ji et al. [22] obtained the graphs with minimal and maximal matching energy. In [6], Chen and Shi obtained tricyclic graph with maximum matching energy. For the unicyclic and bicyclic graphs with a given diameter, Chen et al. [7] obtained the graphs with minimal matching energies. For more results about matching energy, see [4, 5, 8, 24, 25, 28, 29], and see [15] for a survey.

Recall that a matching in a graph is a set of pairwise nonadjacent edges. If M is a matching, the two ends of each edge of M are said to be matched under M, and each vertex incident with an edge of M is said to be covered by M. A *maximum matching* is one which covers as many vertices as possible. The number of edges in a maximum matching of a graph G is called the *matching number* of G and denoted by $\alpha'(G)$. Let $\mathcal{B}(n,\beta)$ and $\mathcal{UB}(n,\beta)$ be the set of connected bipartite graphs and connected bipartite unicyclic graphs with order n and matching number β, respectively. In this paper, we characterize graphs with the first three largest matching energies in $\mathcal{B}(n,\beta)$. Also we determine the extremal graph with minimal and the second minimal matching energy among graphs in $\mathcal{B}(n,\beta)$, respectively. Furthermore, we study the graphs in $\mathcal{UB}(n,\beta)$, and characterize the extremal graph obtaining minimal matching energy.

2 Preliminary

We first introduce some elementary notations and terminology that will be used in the sequel.

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. For a vertex $v \in V(G)$, the *degree* of v is the number of edges of G incident with v. A vertex is called a *k-degree vertex* if its degree is k. In particular, a vertex is called an *isolated vertex* if its degree is zero. A *pendent vertex* is a vertex whose degree is 1. Denote by $N_G(v)$ (or simply $N(v)$) the set of neighbors of v. For a graph G, let $[G]$ be the graph obtained from G by deleting all the isolated vertices of G. For an edge $e = uv \in E(G)$, let $V(e)$ be the set of ends of e, i.e. $V(e) = \{u, v\}$.

A graph H is called a *subgraph* of a graph G if $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. The subgraph of G whose vertex set is X and whose edge set is the set of those edges of G that have both ends in X is called the subgraph of G *induced* by X and is denoted by $G[X]$. For two disjoint sets X, $Y \subseteq V(G)$, let $E(X,Y)$ be the set of edges with one end in X and the other end in Y. For a subset V' of $V(G)$, let $G - V'$ be the subgraph of G obtained by deleting the vertices of V' together with their incident edges. If $V' = \{v\}$, we write $G - v$ instead of $G - \{v\}$. Similarly, for a subset E' of $E(G)$, denote by $G - E'$ the subgraph of G obtained by deleting the edges of E'. If $E' = \{e\}$, we write $G - e$ for $G - \{e\}$. For any two nonadjacent vertices x and y of graph G, let $G + xy$ be the graph obtained from G by adding an edge xy. The *union* of two graphs G and H, denoted by $G \cup H$, is the graph with vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H)$. In particular, if G and H are vertex-disjoint graphs, then denote by $G \uplus H$ the union of G and H. Denote by kG the union of k vertex-disjoint graphs isomorphic to G.

A *bipartite graph* is the graph whose vertex set can be partitioned into two subsets X and Y such that every edge has one end in X and the other end in Y; such a partition (X,Y) is called a *bipartition* of the graph, X and Y its *parts*. Denote by $G[X,Y]$ a bipartite graph G with bipartition (X,Y). If $G[X,Y]$ is simple and every vertex in X is joined to every vertex in Y, then we call G a *complete bipartite graph*. A *star* is a complete bipartite graph $G[X,Y]$ with $|X| = 1$ or $|Y| = 1$. Denote by K_n and S_n the complete graph and the star on n vertices, respectively.

By convention, denote by P_n, C_n the path and the cycle of order n, respectively. A connected graph with n vertices and n edges is called a *unicyclic graph*. For other undefined notations and terminology, we refer the standard textbooks of Bondy and Murty [1,2].

Before stating our main results, we will list or prove some lemmas, which will play an important role in the next proofs.

Lemma 2.1 ([11,14]) *Let G be a simple graph. Then, for any edge $e = uv$ and $N(u) = \{v_1(= v), v_2, \ldots, v_t\}$, we have the following two identities:*

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

$$m(G,k) = m(G-u,k) + \sum_{i=1}^{t} m(G-u-v_i,k-1). \tag{2}$$

Remark 1. According to Eq.(2), we can get $m(P_1 \uplus G, k) = m(G,k)$ directly, where G is an arbitrary graph and P_1 is an isolated vertex. Hence by applying Eq.(2) repeatly, we can deduce that $m(G,k) = m([G],k)$.

Lemma 2.2 ([7]) *Let G be a simple graph and H a subgraph (resp. proper subgraph) of G. Then $G \succeq H$ (resp. $\succ H$).*

Lemma 2.3 ([16]) *Let H_1 and H_2 be two graphs with $H_1 \succ H_2$. Then $H_1 \uplus G \succ H_2 \uplus G$, where G is an arbitrary graph.*

For two non-negative integers n and β with $\beta \leq \frac{n}{2}$, let $\mathcal{T}(n,\beta)$ be the set of trees with order n and matching number β. Denote by $S(n,\beta)$ the graph obtained from $K_{1,\beta-1}$ by attaching one pendent edge to each non-center vertex of $K_{1,\beta-1}$ and attaching $n-2\beta+1$ pendent edges to the center vertex of $K_{1,\beta-1}$. We call the vertex with maximum degree the *center* of $S(n,\beta)$. Let $R(n,\beta)$ be the graph obtained from $S(n-2,\beta-1)$ by attaching an end vertex of a P_3 to a 2-degree vertex of $S(n-2,\beta-1)$ (see Fig. 2.1). We can check that $\alpha'(S(n,\beta)) = \alpha'(R(n,\beta)) = \beta$, which implies $S(n,\beta), R(n,\beta) \in \mathcal{T}(n,\beta)$. In [19], Hou investigated the maching energy of graphs in $\mathcal{T}(n,\beta)$ and gave the following two results.

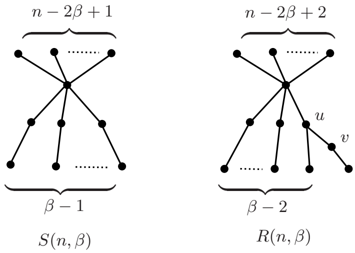

Figure 2.1. The trees with minimal and the second minimal matching energies in $\mathcal{T}(n,\beta)$

Lemma 2.4 ([19]) *Let T be a tree with matching number β, then $T \succeq S(n,\beta)$, with equality holding if and only if $T \cong S(n,\beta)$.*

Lemma 2.5 ([19]) *Let T be a tree with matching number β. If $T \ncong S(n,\beta)$, then $T \succeq R(n,\beta)$, with equality holding if and only if $T \cong R(n,\beta)$.*

3 The graphs with the first three largest matching energies in $\mathcal{B}(n,\beta)$

Note that $\mathcal{B}(n,1) = \{S_n\}$, and $\mathcal{B}(4,2) = \{C_4, P_4\}$, the problem of characterizing extremal graphs with maximal matching energies is trivial in these two cases. Hence, we mainly study graphs in $\mathcal{B}(n,\beta)$ for $n \geq 5$ and $\beta \geq 2$ in this section.

A *covering* of a graph G is a vertex subset $K \subseteq V(G)$ such that each edge of G has at least one end in the set K. The number of vertices in a minimum covering of a graph G is called the *covering number* of G.

Lemma 3.1 (The König-Egerváry Theorem, [10,23]). *In any bipartite graph, the number of edges in a maximum matching is equal to the number of vertices in a minimum covering.*

Let $G = G[X,Y]$ be a bipartite graph such that $G \in \mathcal{B}(n,\beta)$. If $|X| \neq \beta$ and $|Y| \neq \beta$, we then construct a new graph G^* in the following. Firstly, we give some notations that will be used. Let S be a minimum covering of G and $X_1 = S \cap X$, $Y_1 = S \cap Y$. From Lemma 3.1, we know that $|S| = |X_1| + |Y_1| = \beta$. Set $X_2 = X \setminus X_1$, $Y_2 = Y \setminus Y_1$. Clearly, we have $E(X_2, Y_2) = \emptyset$. Since $|X| = |X_1| + |X_2| > \beta$ and $|Y| = |Y_1| + |Y_2| > \beta$, we have that $|Y_2| > |X_1|$ and $|X_2| > |Y_1|$. Then we construct the graph G^* as follows:

$$G^* = G - E(X_1, Y_1) + \{uw : u \in X_1, w \in X_2\}.$$

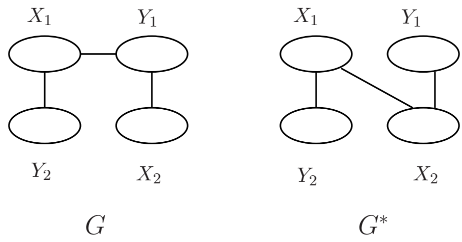

Figure 3.2. The graphs G and G^*

Lemma 3.2 *Let G and G^* be the graphs defined above (see Figure 3.2). Then we have*

$$G^* \succ G.$$

Proof. Let $M_k(G)$ denote the set of k-matchings of G, where $0 \leq k \leq \beta$. Then $m(G,k) = |M_k(G)|$. For any $M \in M_k(G)$, let $M_1 = M \cap E(X_1,Y_2)$, $M_2 = M \cap E(X_2,Y_1)$, and $M_3 = M \cap E(X_1,Y_1)$. If $M_3 = \emptyset$, set $M' = M$. We have that M' is a k-matching of G^*. If $M_3 \neq \emptyset$, suppose that $M_3 = \{x_iy_i : x_i \in X_1, y_i \in Y_1, 1 \leq i \leq t\}$, where $1 \leq t \leq k$. set $Y_1' = V(M_2) \cap Y_1$ and $X_2' = V(M_2) \cap X_2$. Clearly, $\{y_1, y_2, \ldots, y_t\} \subseteq Y_1 \setminus Y_1'$. Since $|X_2| \geq |Y_1|$, we have that $|X_2 \setminus X_2'| \geq |Y_1 \setminus Y_1'|$. Hence, there exists an injection ϕ from the set of t-subsets of $Y_1 \setminus Y_1'$ to the set of t-subsets of $X_2 \setminus X_2'$. Suppose that $\{z_1, z_2, \ldots, z_t\}$ is the image of $\{y_1, y_2, \ldots, y_t\}$ under the injection ϕ. Let $M' = M \cup \{x_1z_1, x_2z_2, \ldots, x_tz_t\} \setminus \{x_1y_1, x_2y_2, \ldots, x_ty_t\}$. Then M' is a k-matching of G^*. Thus we can define a map Φ from $M_k(G)$ to $M_k(G^*)$ which maps M to M'. From the construction of M', we know that Φ is an injection. Hence, $m(G^*,k) \geq m(G,k)$. Moreover, we know that $m(G^*,1) > m(G,1)$. Thus, $G^* \succ G$. ■

Lemma 3.2 is an efficient tool for the characterization of the graphs with the first three largest matching energies among graphs in $\mathcal{B}(n,\beta)$. Although the maximum matching energy among all bipartite graphs with a given matching number has already been determined in [9], we will give our proof using Lemma 3.2 in the following.

Theorem 3.3 *Among all the graphs in $\mathcal{B}(n,\beta)$, $K_{\beta,n-\beta}$ is the unique graph with maximal matching energy.*

Proof. Let G be a graph with matching number β and $G \ncong K_{\beta,n-\beta}$. The result $K_{\beta,n-\beta} \succ G$ holds trivially for $|X| = \beta$ or $|Y| = \beta$. Now we consider $|X| > \beta$ and $|Y| > \beta$. From Lemma 3.2, we know that $G^* \succ G$, where G^* is the graph obtained from G by the operation shown in Fig. 3.2. Since G^* is a subgraph of $K_{\beta,n-\beta}$, we have $K_{\beta,n-\beta} \succeq G^*$. Hence, $K_{\beta,n-\beta} \succ G$. The result follows. ■

From Lemma 3.2 and Theorem 3.3, we can get the following result.

Theorem 3.4 *Among all the graphs in $\mathcal{B}(n,\beta)$, $K_{\beta,n-\beta} - e$ is the unique graph with the second maximal matching energy, where e is an arbitrary edge of $K_{\beta,n-\beta}$.*

Proof. Suppose that $G \in \mathcal{B}(n,\beta)$ is the graph with the second maximal matching energy. Let (X,Y) be the bipartition of G. We claim that either $|X| = \beta$ or $|Y| = \beta$. Otherwise, let G^* be the graph obtained from G by the operation shown in Fig. 3.2. From Lemma 3.2, we know that $G^* \succ G$. Note that the bipartition of G^* is $(X_1 \cup Y_1, X_2 \cup Y_2)$ and $|X_1| + |Y_1| = \beta$. Since $|X| = |X_1| + |X_2| > \beta$ and $|Y| = |Y_1| + |Y_2| > \beta$, we have that $|X_2| > |Y_1|$ and $|Y_2| > |X_1|$. In addition, we can get that $|X_1| \geq 1$ and $|Y_1| \geq 1$ by the connectedness of G. So $|X_2| \geq 2$ and $|Y_2| \geq 2$. Hence, $G^* \ncong K_{\beta,n-\beta}$, and so $K_{\beta,n-\beta} \succ G^* \succ G$, a contradiction. The claim follows. From Lemma 2.2 and Theorem 3.3, one can see that the graph obtained from $K_{\beta,n-\beta}$ by deleting an arbitrary edge is the unique graph with the second maximal matching energy among all the graphs in $\mathcal{B}(n,\beta)$.
■

Theorem 3.5 *Among all the graphs in $\mathcal{B}(n,\beta)$, $K_{\beta,n-\beta} - e_1 - e_2$ is the unique graph with the third maximal matching energy, where e_1 and e_2 are two arbitrary nonadjacent edges of $K_{\beta,n-\beta}$.*

Proof. Suppose that $G \in \mathcal{B}(n,\beta)$ is the graph with the third maximal matching energy. Let (X,Y) be the bipartition of G. We claim that either $|X| = \beta$ or $|Y| = \beta$. Otherwise, let G^* be the graph obtained from G by the operation shown in Fig. 3.2. Then by the similar argument in the proof of Theorem 3.4, we can get that $|Y_2| \geq 2$ and $|Y_1| \geq 1$. Hence, $G^* \ncong K_{\beta,n-\beta}$, and $G^* \ncong K_{\beta,n-\beta} - e$, where e is an arbitrary edge of $K_{\beta,n-\beta}$. So we have that $K_{\beta,n-\beta} \succ K_{\beta,n-\beta} - e \succ G^* \succ G$, a contradiction. The claim follows.

From Lemma 2.2, Theorems 3.3 and 3.4, we can get that G can be obtained from $K_{\beta,n-\beta}$ by deleting two edges. Let $X = \{x_1, x_2, \ldots, x_\beta\}$ and $Y = \{y_1, y_2, \ldots, y_{n-\beta}\}$ be the bipartition of $K_{\beta,n-\beta}$. Let $G' = K_{\beta,n-\beta} - x_1y_1 - x_1y_2$ and $G'' = K_{\beta,n-\beta} - x_1y_1 - x_2y_2$. Up to isomorphism, the graph obtained from $K_{\beta,n-\beta}$ by deleting two edges is G' or G''. Clearly, $G'' - x_1y_2 \cong G' - x_2y_2 \cong K_{\beta,n-\beta} - x_1y_1 - x_1y_2 - x_2y_2$, $G'' - x_1 - y_2 \cong K_{\beta-1,n-\beta-1}$

and $G' - x_2 - y_2 \cong K_{\beta-1,n-\beta-1} - x_1y_1$. Hence, for $2 \le k \le \beta$,

$$\begin{aligned} m(G'', k) &= m(G'' - x_1y_2, k) + m(G'' - x_1 - y_2, k-1) \\ &> m(G' - x_2y_2, k) + m(G' - x_2 - y_2, k-1) \\ &= m(G', k). \end{aligned}$$

Together with $m(G'', 1) = m(G', 1)$, we have that $G'' \succ G'$. Hence, $G \cong G''$. The result follows. ■

4 The extremal graphs with minimal and the second minimal matching energy in $\mathcal{B}(n, \beta)$

In this section, we study the graphs in $\mathcal{B}(n, \beta)$, and characterize the extremal graphs with minimal and the second minimal matching energies, respectively.

Theorem 4.1 *Let G be a graph in $\mathcal{B}(n, \beta)$. If $G \ncong S(n, \beta)$, then $ME(G) > ME(S(n, \beta))$.*

Proof. Suppose that G is a graph in $\mathcal{B}(n, \beta)$, and $G \ncong S(n, \beta)$. If G contains no cycle, then $G \in \mathcal{T}(n, \beta)$. Hence, $G \succ S(n, \beta)$ by applying Lemma 2.4.

We then suppose that G contains cycles. There must exist an edge $e_1 \in E(G)$ such that $G - e_1$ is connected and $\alpha'(G - e_1) = \alpha'(G) = \beta$. If $G - e_1$ is a tree, by Lemmas 2.2 and 2.4, we can get $G \succ G - e_1 \succeq S(n, \beta)$. If $G - e_1$ also contains cycles, we can find an edge e_2 of $G - e_1$ similarly to the above operation such that $G - e_1 - e_2 \in \mathcal{B}(n, \beta)$ and $G \succ G - e_1 - e_2$. Repeat the operation, one can get a spanning subgraph T of G such that $T \in \mathcal{B}(n, \beta)$ and $G \succ T \succeq S(n, \beta)$ finally.

We have proved that $G \succ S(n, \beta)$ in both cases. Therefore, one can get $ME(G) > ME(S(n, \beta))$ by Eq. (4). ■

From Theorem 4.1, we have that $S(n, \beta)$ is the extremal graph with minimal matching energy in $\mathcal{B}(n, \beta)$. Then we start to characterize the extremal graph with the second minimal matching energy in $\mathcal{B}(n, \beta)$.

Denote by $UB(n, \beta)$ the unicyclic graph shown in Figure 4.3.

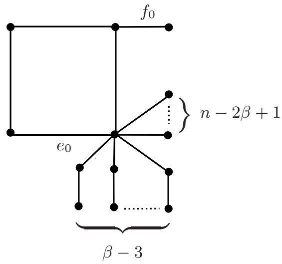

Figure 4.3. The graph $UB(n,\beta)$.

Theorem 4.2 *Let G be a graph in $\mathcal{B}(n,\beta)$. If $G \ncong S(n,\beta)$ or $R(n,\beta)$, then $ME(G) > ME(R(n,\beta))$.*

Proof. Suppose that G is a graph in $\mathcal{B}(n,\beta)$, and $G \notin \{S(n,\beta), R(n,\beta)\}$. If G contains no cycle, then $G \in \mathcal{T}(n,\beta)$. Hence, we have $G \succ R(n,\beta)$ applying Lemmas 2.4 and 2.5.

Suppose that G contains cycles. Then we aim to find a unicyclic spanning subgraph H of G such that $H \in \mathcal{B}(n,\beta)$. Clearly, $H \cong G$ if G is a unicyclic graph. If G contains at least two cycles, then there must exist an edge e_1 in G such that $G - e_1 \in \mathcal{B}(n,\beta)$ and $G - e_1$ contains at least one cycle. If $G - e_1$ also contains at least two cycles, we can find an edge e_2 of $G - e_1$ similarly to the above operation such that $G - e_1 - e_2 \in \mathcal{B}(n,\beta)$ and $G \succ G - e_1 - e_2$. Repeat the operation, one can get a unicyclic spanning subgraph H of G such that $H \in \mathcal{B}(n,\beta)$ finally.

Since H is a unicyclic graph, there must exist an edge e of the cycle in H such that $H - e \in \mathcal{B}(n,\beta)$. If $H - e \ncong S(n,\beta)$, then by Lemmas 2.2 and 2.5, we can get $G \succeq H \succ H - e \succeq R(n,\beta)$.

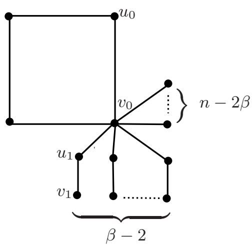

Figure 4.4. The graph G_1.

If $H - e \cong S(n,\beta)$, then H is isomorphic to $UB(n,\beta)$ or G_1(see Figure 4.4). If $H \cong UB(n,\beta)$, then $H - e_0 \cong R(n,\beta)$. Thus we can get $H \succ H - e_0 \cong R(n,\beta)$ from

Lemma 2.2. If $H \cong G_1$, then $H \succ H - u_0v_0 \succ R(n, \beta)$. Therefore, we can always obtain that $G \succeq H \succ R(n, \beta)$. Hence, we complete the proof. ■

5 The extremal graph with minimal matching energy in $\mathcal{UB}(n, \beta)$

Recall that $\mathcal{UB}(n, \beta)$ is the set of unicyclic bipartite graphs with order n and matching number β.

Note that the graphs G_1 (see Fig. 4.4) and $UB(n, \beta)$ play an important role in the proof of Theorem 4.2 and both these two graphs belong to $\mathcal{UB}(n, \beta)$. Motivated by the result $G_1 \succ UB(n, \beta)$ which is obtained from simple comparation, we begin to characterize the extremal graph with minimal matching energy among the graph class $\mathcal{UB}(n, \beta)$.

Lemma 5.1 *Let $G \in \mathcal{UB}(n, \beta)$ ($\beta < \frac{n}{2}$) with the unique cycle C. If there exists an edge $e \in E(C)$ such that $G - e \cong S(n, \beta)$ or $R(n, \beta)$, then $G \succ UB(n, \beta)$ unless $G \cong UB(n, \beta)$.*

Proof. Suppose that $G \ncong UB(n, \beta)$. Then it is sufficient to prove that $G \succ UB(n, \beta)$. If there exists an $e \in E(C)$ such that $G - e \cong S(n, \beta)$, then G is isomorphic to G_1 (see Fig. 4.4). Since $G - u_1v_1 \cong UB(n, \beta) - f_0$ and $G - u_1 - v_1 \supset UB(n, \beta) - V(f_0)$, we have

$$\begin{aligned} m(G, k) &= m(G - u_1v_1, k) + m(G - u_1 - v_1, k - 1) \\ &\geq m(UB(n, \beta) - f_0, k) + m(UB(n, \beta) - V(f_0), k - 1) \\ &= m(UB(n, \beta), k). \end{aligned}$$

Since $G - u_1 - v_1 \supset UB(n, \beta) - V(f_0)$, there exists k_0 such that $m(G - u_1 - v_1, k_0) > m(UB(n, \beta) - V(f_0), k_0)$, and so $m(G, k_0 + 1) > m(UB(n, \beta), k_0 + 1)$. Hence, $G \succ UB(n, \beta)$.

If there exists an edge $e \in E(C)$ such that $G - e \cong R(n, \beta)$, then G is isomorphic to G_i, $i = 2, 3, \ldots, 9$ (see Fig. 5.5).

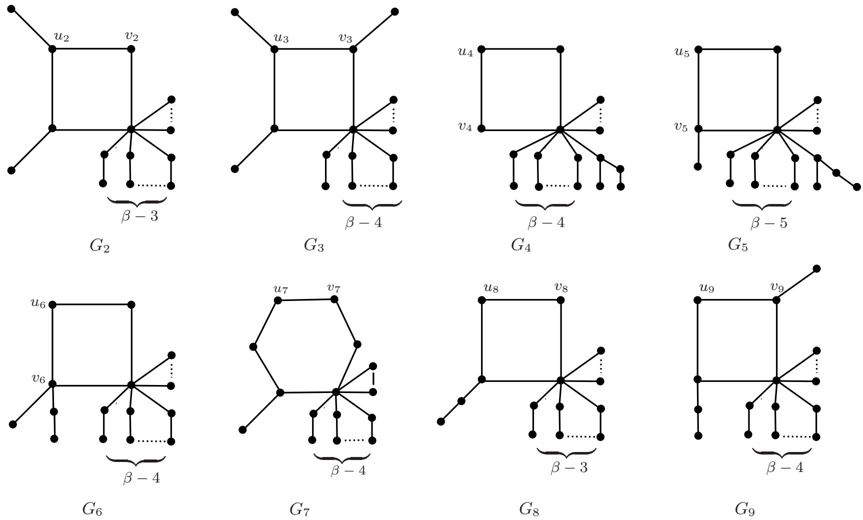

Figure 5.5. The graphs G_2 to G_9.

Clearly, $UB(n,\beta) - e_0 \cong R(n,\beta)$. For $2 \leq i \leq 9$, we can find that $G_i - u_iv_i \in \mathcal{T}(n,\beta) \setminus S(n,\beta)$. Then $G_i - u_iv_i \succeq UB(n,\beta) - e_0$ from Lemmas 2.4 and 2.5. Since $[UB(n,\beta) - V(e_0)] \cong (\beta-3)P_2 \uplus P_3$ and $G - u_i - v_i \supset (\beta-3)P_2 \uplus P_3$, we have $G_i - u_i - v_i \succ UB(n,\beta) - V(e_0)$. Therefore, we can get that

$$
\begin{aligned}
m(G_i,k) &= m(G_i - u_iv_i, k) + m(G_i - u_i - v_i, k-1) \\
&\geq m(UB(n,\beta) - e_0, k) + m(UB(n,\beta) - V(e_0), k-1) \\
&= m(UB(n,\beta), k).
\end{aligned}
$$

Since $G - u_i - v_i \succ UB(n,\beta) - V(e_0)$, there exists k_0 such that $m(G_i - u_i - v_i, k_0) > m(UB(n,\beta) - V(e_0), k_0)$, and so $m(G_i, k_0+1) > m(UB(n,\beta), k_0+1)$. Hence, $G \succ UB(n,\beta)$. ■

Lemma 5.2 *Suppose that $G \in \mathcal{UB}(n,\beta)$ with the unique cycle C. If there exists a maximum matching M of G such that $M \cap E(C) \neq \emptyset$, then we have $G \succ UB(n,\beta)$ unless $G \cong UB(n,\beta)$.*

Proof. Suppose that $C = v_1v_2\dots v_s$ and $v_iv_{i+1} \in M \cap E(C)$. Then $G - v_iv_{i-1} \in \mathcal{T}(n,\beta)$. If $G - v_iv_{i-1} \cong S(n,\beta)$ or $R(n,\beta)$, then $G \succ UB(n,\beta)$ by Lemma 5.1. We suppose in the following that $G - v_iv_{i-1} \ncong S(n,\beta)$ and $R(n,\beta)$. By Lemmas 2.4 and 2.5, we have $G - v_iv_{i-1} \succ R(n,\beta) = UB(n,\beta) - e_0$.

If $\alpha'(G - v_i - v_{i-1}) = \beta - 1$, then $G - v_i - v_{i-1} \supseteq (\beta-1)P_2$. It is easy to check that $P_2 \uplus P_2 \succ P_3$. Thus from Lemma 2.3, $(\beta-1)P_2 \succ (\beta-3)P_2 \uplus P_3 \cong [UB(n,\beta) - V(e_0)]$. Hence $G - v_i - v_{i-1} \succ UB(n,\beta) - V(e_0)$. If $\alpha'(G - v_i - v_{i-1}) = \beta - 2$, then $M \setminus \{v_i, v_{i-1}\}$ is a $(\beta-2)$-matching of $G - v_i - v_{i-1}$. Since v_{i+1} is not matched in $M \setminus \{v_i, v_{i-1}\}$, and v_{i+1} is not isolated in $G - v_i - v_{i-1}$, we have that $G - v_i - v_{i-1} \supseteq (\beta-3)P_2 \uplus P_3 \cong [UB(n,\beta) - V(e_0)]$ which implies that $G - v_i - v_{i-1} \succeq UB(n,\beta) - V(e_0)$. Therefore, we can get

$$\begin{aligned} m(G,k) &= m(G - v_iv_{i-1}, k) + m(G - v_i - v_{i-1}, k-1) \\ &\geq m(UB(n,\beta) - e_0, k) + m(UB(n,\beta) - V(e_0), k-1) \\ &= m(UB(n,\beta), k). \end{aligned}$$

Since $G - v_iv_{i-1} \succ UB(n,\beta) - e_0$, there exists k_0 such that $m(G - v_iv_{i-1}, k_0) > m(UB(n,\beta) - e_0, k_0)$. Then $m(G, k_0) > m(UB(n,\beta), k_0)$. Hence $G \succ UB(n,\beta)$. ∎

Let G be an unicyclic graph with the unique cycle C. For a vertex $v \in V(C)$, denote by T_v the component of $G - E(C)$ containing v.

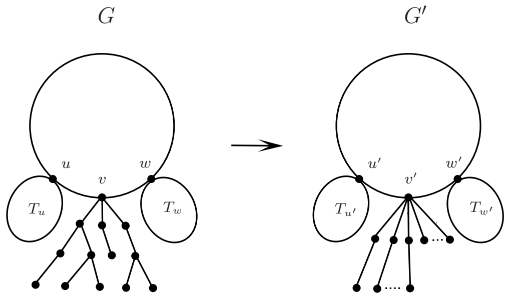

Figure 5.6. Replace T_v with $S(n(T_v), \alpha'(T_v))$.

Lemma 5.3 *Suppose that $G \in \mathcal{UB}(n,\beta)$ with the unique cycle C such that $M \cap E(C) = \emptyset$ for any maximum matching M of G. Let G' be the graph obtained from G by replacing T_v with $S(n(T_v), \alpha'(T_v))$, and identifying vertex v with the center of $S(n(T_v), \alpha'(T_v))$, where $n(T_v)$ and $\alpha'(T_v)$ are the order and matching number of T_v (See Figure 5.6). Then we have $G' \in \mathcal{UB}(n,\beta)$ and $G \succ G'$ unless $T_v \cong S(n(T_v), \alpha'(T_v))$.*

Proof. Let $u(u')$ and $w(w')$ be two neighbors of $v(v')$ in the unique cycle of $G(G')$. Since the maximum matching of G contains no edges of C, $\alpha'(G) = \alpha'(G - T_v) + \alpha'(T_v)$. Let

M' be a maximum matching of G'. If M' contains edge $u'v'$ or $v'w'$, suppose without loss of generality that $u'v' \in M'$, then $M' - u'v' + v'x$ is also a maximum matching of G', where x is a pendent vertex adjacent to v' in $T_{v'}$ (such a vertex x must exist from the definition of graph $S(n(T_v), \alpha'(T_v))$). Hence, there exists a maximum matching of G' not containing edges $u'v'$ and $v'w'$, which implies that $\alpha'(G') = \alpha'(G' - T_{v'}) + \alpha'(T_{v'})$. Since $G - T_v \cong G' - T_{v'}$ and $\alpha'(T_v) = \alpha'(T_{v'})$, one can deduce that

$$\alpha'(G') = \alpha'(G' - T_{v'}) + \alpha'(T_{v'}) = \alpha'(G - T_v) + \alpha'(T_v) = \alpha'(G) = \beta.$$

Therefore, $G' \in \mathcal{UB}(n, \beta)$.

If $T_v \ncong S(n(T_v), \alpha'(T_v))$, by Lemma 2.4, one can get that $T_v \succ T_{v'}$. Hence for any $k \geq 0$, one can have the following result by Lemmas 2.1 and 2.3:

$$\begin{aligned}
m(G,k) &= m(G - vw, k) + m(G - v - w, k-1) \\
&= m(G - vw - uv, k) + m(G - vw - u - v, k-1) + m(G - v - w, k-1) \\
&= m((G - T_v) \cup T_v, k) + m((G - T_u - T_v) \cup (T_u - u) \cup (T_v - v), k-1) \\
&\quad + m((G - T_v - T_w) \cup (T_v - v) \cup (T_w - w), k-1) \\
&\geq m((G' - T_{v'}) \cup T_{v'}, k) + m((G' - T_{u'} - T_{v'}) \cup (T_{u'} - u') \cup (T_{v'} - v'), k-1) \\
&\quad + m((G' - T_{v'} - T_{w'}) \cup (T_{v'} - v') \cup (T_{w'} - w'), k-1) \\
&= m(G' - v'w' - u'v', k) + m(G' - v'w' - u' - v', k-1) \\
&+ m(G' - v' - w', k-1) = m(G' - v'w', k) + m(G' - v' - w', k-1) \\
&= m(G', k).
\end{aligned}$$

Since $T_v \succ T_{v'}$, by Lemma 2.3, we have that $(G - T_v) \cup T_v \succ (G' - T_{v'}) \cup T_{v'}$. Then there exists k_0 such that $m((G - T_v) \cup T_v, k_0) > m((G' - T_{v'}) \cup T_{v'}, k_0)$, and so $m(G, k_0) > m(G', k_0)$. Hence, $G \succ G'$. ■

Theorem 5.4 *Among all the graphs in $\mathcal{UB}(n, \beta)$ ($\beta < \frac{n}{2}$), $UB(n, \beta)$ is the unique graph with minimal matching energy.*

Proof. Suppose that $G \ncong UB(n, \beta)$ and C is the unique cycle of G. Then it is sufficient to prove that $G \succ UB(n, \beta)$. If there exists an edge $e \in E(C)$ such that $G - e \in \{S(n, \beta), R(n, \beta)\}$, we have $G \succ UB(n, \beta)$ from Lemma 5.1. Hence, we suppose that for any edge $e \in E(C)$, $G - e \notin \{S(n, \beta), R(n, \beta)\}$.

If there exists a maximum matching M of G such that $M \cap E(C) \neq \emptyset$, then the result holds from Lemma 5.2. Then we consider the case that $M \cap E(C) = \emptyset$ for any maximum matching M of G.

We claim that T_v is not trivial for any vertex $v \in V(C)$. If not, there is a vertex $v_0 \in V(C)$ such that T_{v_0} is trivial, that is, T_{v_0} contains only one vertex v_0. Let u_0 and w_0 be the neighbors of v_0 on C. Then any maximum matching M of G does not contain the edge u_0v_0 or v_0w_0. By the maximality of M, we have that at least one of the vertices u_0 and w_0 is covered by M. Without loss of generality, suppose that u_0 is covered by M and $u_0p_0 \in M$. Let $M' = M \cup u_0v_0 \setminus u_0p_0$. Then M' is a maximum matching of G and $M' \cap E(C) \neq \emptyset$, a contradiction. The claim follows.

For any vertex $v \in V(C)$, replacing T_v with $S(n(T_v), \alpha'(T_v))$, and identifying vertex v with the center of $S(n(T_v), \alpha'(T_v))$. Denoted the resulting graph by G'. From Lemma 5.3, we know that $G' \in \mathcal{UB}(n, \beta)$ and $G \succeq G'$. From the above claim, we know that v is incident with at least one pendent edge in G'. Since $\beta < \frac{n}{2}$, that is, G' has no perfect matching, there exists a vertex $v_i \in V(C)$ such that v_i is adjacent to at least 2 pendent vertices, say w_1 and w_2. By the assumption, we have $G - v_{i+1}v_{i+2} \in \mathcal{T}(n, \beta)$, and $G - v_{i+1}v_{i+2} \succ R(n, \beta) \cong UB(n, \beta) - e_0$.

If $\alpha'(G - v_{i+1} - v_{i+2}) = \beta - 1$, then we can get $G - v_{i+1} - v_{i+2} \succ UB(n, \beta) - V(e_0)$. If $\alpha'(G - v_{i+1} - v_{i+2}) = \beta - 2$, we have $G - v_{i+1} - v_{i+2} \supseteq (\beta - 3)P_2 \uplus P_3 \cong [UB(n, \beta) - V(e_0)]$, where $P_3 = w_1v_iw_2$. Hence we can obtain that $G - v_{i+1} - v_{i+2} \succeq UB(n, \beta) - V(e_0)$ in both cases.

Therefore, we have

$$\begin{aligned} m(G, k) &= m(G - v_{i+1}v_{i+2}, k) + m(G - v_{i+1} - v_{i+2}, k - 1) \\ &\geq m(UB(n, \beta) - e_0, k) + m(UB(n, \beta) - V(e_0), k - 1) \\ &= m(UB(n, \beta), k). \end{aligned}$$

Since $G - v_{i+1}v_{i+2} \succ UB(n, \beta) - e_0$, there exists k_0 such that $m(G - v_{i+1}v_{i+2}, k_0) > m(UB(n, \beta) - e_0, k_0)$. Then $m(G, k_0) > m(UB(n, \beta), k_0)$. Hence $G \succ UB(n, \beta)$. ■

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