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Two Graph Transformations and Their Applications to Matching Theory of Graphs*

Hailiang Zhang[1], Lu Liu[2]

[1]*Department of Mathematics, Taizhou University*
Lin Hai, 317000, P. R. China

hdsdzhl@163.com

[2]*College of public basic sciences, Jinzhou Medical University,*
Jinzhou, 121000, P. R. China

lulu4101112@163.com

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Abstract

In this note we study the behavior of largest matching root, Hosoya index and matching energy under two graph structural transformations. As an application we characterize the extremal graphs with respect to the largest matching root, matching energy, and Hosoya index, of graphs with cyclomatic number one, two, and three. We also give numerical bounds for each above graph parameters.

1 Introduction

All graphs considered in this paper are undirected, connected and simple (i.e., loops and multiple edges are not allowed). Let $G = (V(G), E(G))$ be a graph with a vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and an edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$, where $e(G) = n$ is the *order* and $e(G) = m$ is the *size* of G. Let $\Gamma_G(v)$ denote the neighbor set of vertex v of G. Two edges are called *adjacent* if they have a common vertex. A *matching* M is a subset of $E(G)$ where no two edges of M are adjacent. Let $\mathcal{M}(G, k)$ denote matchings have

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k edges, and $m(G,k)$ denote the number of k-matchings of G. Farrell [4], Gutman [8] denoted the *matching polynomial* as

$$M_G(x) = \sum_{k\geq 0}^{n/2} (-1)^k m(G,k) x^{n-2k}. \tag{1.1}$$

In addition, we set $m(G,0) = 1$ by convention. Obviously, $m(G,1) = e(G)$, and $m(G,k) = 0$ if $k > n/2$.

Let $\theta_n \leq \theta_{n-1} \leq \ldots \leq \theta_2 \leq \theta_1 = \theta(G)$ be the roots of matching polynomial of G, and $\theta(G)$ be the largest matching root. It is obvious that the matching roots are symmetric to 0. Heilmann and Leib [1], I. Gutman [2], and C. D. Godsil [6], proved that the roots of matching polynomial of graphs are real. Godsil [6] also proved that if G has a Hamilton path then G has no repeat roots, and the number of distinct matching roots at least equals to the diameter of G plus one. For all graphs the largest matching root satisfy

$$\theta(P_n) \leq \theta(G) \leq \theta(K_n), \tag{1.2}$$

where P_n, K_n denote path and complete graph on n vertices, and $\theta(P_n) = 2\cos(\pi/(n+1))$. The largest matching root of K_n can not be expressed by radicals.

Hosoya [3] studied the summation of absolute of all coefficients of matching polynomial of a graph, that is

$$Z(G) = \sum_{k=0}^{n/2} |m(G,k)|. \tag{1.3}$$

In many literature, $Z(G)$ is called Hosoya index. It is proved that for trees,

$$n = Z(K_{1,n}) < Z(T) < Z(P_n) = f_{n+1}, \tag{1.4}$$

where f_n is the n-th Fibonacci number.

Gutman and Wager in [7] proposed the concept of matching energy of a graph, which is the sum of absolute value of all matching roots of G, also denoted by

$$ME(G) = \frac{2}{\pi}\int_0^{\infty} \frac{1}{x^2} \ln(\sum_{k\geq 0} m(G,k)x^{2k})dx. \tag{1.5}$$

By this definition, we can deduce that if $m(G,k) \geq m(H,k)$ for every $k \geq 1$, then $ME(G) \geq ME(H)$.

Gutman and F. J. Zhang [9], also Peter [10], et. al. introduced that if $m(G_1,k) \geq m(G_2,k)$ for all k, then G_1 is m-greater than G_2, written as $G_1 \succeq G_2$. If $m(G_1,k) =$

$m(G_2, k)$ then G_1 and G_2 are matching equivalent, written as $G_1 \sim G_2$. If neither $G_1 \succ G_2$ nor $G_2 \succ G_1$, then G_1 and G_2 are m-incomparable.

Let $\mathscr{U}_n$, $\mathscr{B}_n$, $\mathscr{T}_n$ denote unicyclic graphs, bicyclic graphs, and tricyclic graphs of order n, or graphs with cyclomatic number one, two and three, respectively. If $e(G) = n(G) - 1$, then we call G a tree, denoted by T. Gutman [2], [8] , Godsil [5], [6], proved that for trees the largest matching roots and the adjacency spectral radius are the same. H. L. Zhang [11] studied the largest matching root of unicyclic graphs and characterized the extremal graph. W. J. Liu et. al. [12] gave the four largest and the two smallest value for the unicyclic graphs. H. L. Zhang [13] characterized the extremal graph with respect to the largest matching root among unicyclic graphs with a fixed matching number. S. Ji, X. Li, and Y. Shi [14] characterized the extremal matching energy of bicyclic graphs. Lin Chen, Yongtang Shi [15] characterized extremal matching energy of tricyclic Graphs. Xiaolin Chen and Huishu Lian [16] studied the extremal matching energy and the largest matching root of complete multipartite graphs. Form above results we found the largest matching root, Hosoya index and graph matching energy are highly related. Consequently, we may conjecture that

$$G_1 \succeq G_2 \Leftrightarrow Z(G_1) \geq Z(G_2) \Leftrightarrow ME(G_1) \geq ME(G_2) \Leftrightarrow \theta(G_1) \leq \theta(G_2).$$

In this paper, we give two graph transformations related to the matching polynomial of a graph. We present their application to characteristic extremal graphs with respect to the largest matching root, Hosoya index, and graph matching energy, among different classes of graphs. We also give numerical bounds for above graph parameters and partially prove the above Conjecture also true for these types of graphs.

2 Preliminary

Let $G - v$ be the graph obtained by deleting a vertex v with its incident edges form G. $G - e$ be the graph obtained by deleting an edge e from G. The following Lemma 2.1, Lemma 2.2 are often used to calculate the matching polynomial of a graph.

Lemma 2.1 *[8] Let G be a graph with $u \in V(G)$, and suppose the neighborhood of u is $\Gamma(u) = \{v_1, v_2, \ldots, v_k\}$, $uv \in E(G)$. Then*

1. $M_G(x) = M_{G-e}(x) - M_{G-u-v}(x)$,

2. $M_G(x) = xM_{G-u}(x) - \sum_{uv_i \in E(G)} M_{G-u-v_i}(x), v_i \in \Gamma(u).$

Lemma 2.2 *[8] Let $G_1, G_2, \ldots, G_k$ be k components of G. Then*

$$M_G(x) = \prod_{i=1}^{k} M_{G_i}(x).$$

Lemma 2.3 (Interlacing Theorem [2], [5]) *If v is a vertex of G, then the roots of $G - v$ and G has the following inequality*

$$\theta_n(G) \leq \ldots \leq \theta_{i+1}(G) \leq \theta_i(G-v) \leq \theta_i(G) \leq \ldots \leq \theta_1(G).$$

In particular, if G admits a Hamilton path then the above inequality strict.

Lemma 2.4 *[8] Let $v_1, \ldots, v_n$ be the vertices of a graph G, Let $G - v_i$ be the subgraphs of G obtained by deleting the vertex v_i, then*

$$\frac{d}{dx} M_G(x) = \sum_{i=1}^{n} M_{G-v_i}(x) = \sum_{k=0}^{n/2} (-1)^k (n-2k) m(G,k) x^{n-2k-1}. \tag{2.1}$$

Lemma 2.5 *Let G^* be a spanning subgraph of G, $\theta(G)$ be the largest matching root of G. If $x \geq \theta(G)$ then $M_{G^*}(x) \geq M_G(x)$. If G^* is a proper spanning subgraph of G and $x > \theta(G)$, then $\theta(G^*) > \theta(G)$.*

Proof. Let G^* be spanning subgraph of G if not we can add some isolated vertices, and $V(G) = \{v_1, v_2, \ldots, v_n\}$ be the vertex set of G. $G_i = G - v_i$, $G_i^* = G^* - v_i$. For $x \in [\theta(G), \infty)$, we have

$$f(x) = M_{G^*}(x) - M_G(x). \tag{2.2}$$

We need to prove that $f(x) \geq 0$, when $x \geq \theta(G)$. By applying differentiation on Equation (2.2) and with Lemma 2.4 (2.1), we have

$$\begin{aligned} f'(x) &= M'_{G^*}(x) - M'_G(x) = \sum_i M_{G_i^*}(x) - \sum_i M_{G_i}(x) \\ &= \sum_i (M_{G_i^*}(x) - M_{G_i}(x)). \end{aligned} \tag{2.3}$$

Now, we apply induction on the number of vertices.

Case 1 When $n = 1$, the result is trivial.

Case 2 When $n = 2$, $G \cong K_2$, and G^* is empty graph of order 2. Obviously, by the Lemma 2.1 and the Lemma 2.2, we have

$$M_G(x) = x^2 - 1, \quad M_{G^*}(x) = x^2.$$

When $x \geq 1$, $x^2 > x^2 - 1$ holds, so the Lemma 2.5 holds.

Case 3 Assume that the Lemma 2.5 holds when the order of G is less than n. We will show that Lemma 2.5 holds when the order of G is n.

When $n \geq 3$, $|V(G_i)| = n - 1$. For every G_i there exists a spanning subgraph G_i^* correspond to it. By our assumption, $M_{G_i^*}(x) \geq M_{G_i}(x)$ when $x \geq \theta(G_i)$. By the Lemma 2.3, $\theta(G) \geq \max\{\theta(G_1), \ldots, \theta(G_n)\}$. Then for $x \geq \theta(G)$,

$$f'(x) = M'_{G^*}(x) - M'_G(x) = \sum_i (M_{G_i^*}(x) - M_{G_i}(x)) \geq 0,$$

holds. If G^* is a proper spanning subgraph of G, without loss generality, let G_j^* be the proper spanning subgraph of G_j, $(1 \leq j \leq n)$ by our assumption, when $x = \theta(G) > \theta(G_j)$,

$$M_{G_j^*}(x) > M_{G_j}(x).$$

Therefore,

$$f'(x) = M'_{G^*}(x) - M'_G(x) = \sum_i M_{G^*}(x) - \sum_i M_G(x) > 0.$$

That is $f'(\theta(G)) > 0$, and

$$f(\theta(G)) = M_{G^*}(\theta(G)) - M_G(\theta(G)) = M_{G^*}(\theta(G)) > 0.$$

It shows that when $x \geq \theta(G)$, $f(x)$ is a monotonic increasing function. ∎

Since for every subgraph H of G we can add some isolated vertices to H let it be a spanning subgraph of G. Hence, for any subgraph H of G, we have the following Corollary 2.6 and Corollary 2.7.

Corollary 2.6 *For any subgraph H of G, if $x \geq \theta(G)$ then $M_H(x) \geq 0$.*

Corollary 2.7 *For graph G_1 and G_2. If $M_{G_2}(x) \geq M_{G_1}(x)$ for $x \in [\theta(G_1), \infty)$, then $\theta(G_2) \leq \theta(G_1)$.*

Definition 2.8 *[10] Let u, v be two vertices of the graph G, we obtain the Kelmans transformation of G as follows: we erase all edges between v and $N(v) - (N(u) \cup \{u\})$ and add all edges between u and $N(v) - (N(u) \cup \{u\})$. Let us call u and v the beneficiary and the co-beneficiary of the transformation, respectively. The obtained graph has the same number of edges as G; in general we will denote it by G^* without referring to the vertices u and v.(see Fig.1.).*

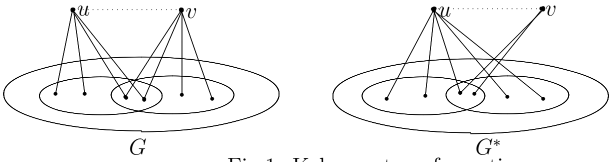

Fig.1. Kelmans transformation

Lemma 2.9 *[10] Assume that G^* is a graph obtained from G by some Kelmans transformation, then*

$$m(G^*,k) \leq m(G,k), 0 \leq k \leq n/2 \quad and \quad \theta(G) \leq \theta(G^*). \tag{2.4}$$

Let G be a simple graph. If $e = (v_1v_2)$ is not an edge of C_3 of G, then $G \diamond e$ denotes the graph obtained by contracting edge e. G^* denotes the graph obtained by adding a pendant edge to the contracted vertex u of $G \diamond e$ (see Fig. 2.). For the largest matching root of G and G^*, we have the following Lemma 2.10. With regard to the perturbation on the largest matching root also see [13].

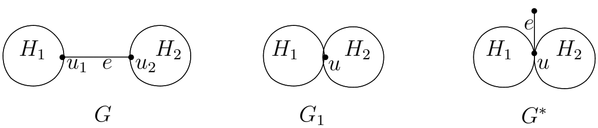

Fig. 2. G, $G \diamond e$ and G^*

Lemma 2.10 *Let H_1 and H_2 be two graphs with distinguished vertices u_1, u_2 of H_1 and H_2, respectively. Let G be the graph connecting u_1 and u_2 by an edge e. Let H_1uH_2 be the graph obtained from H_1 and H_2 by identifying the vertices of u_1 and u_2 to a new vertex u (see G_1 in Fig. 2.). Let G^* be the graph obtained by attaching a pendant to u of G_1 (see G^* in Fig. 2.). Then*

$$m(G^*,k) \leq m(G,k), \; and \quad \theta(G) < \theta(G^*). \tag{2.5}$$

Proof. By Lemma 2.1 and Lemma 2.2, we calculate the matching polynomial of G and G^* as:

$$\begin{aligned} M_G(x) &= M_{H_1}(x)M_{H_2}(x) - M_{H_1-u_1}(x)M_{H_2-u_2}(x) \\ &= (xM_{H_1-u_1}(x) - \sum_{u\in\Gamma_{H_1}(u_1)} M_{H_1-u_1u}(x)) \\ &\quad (xM_{H_2-u_2}(x) - \sum_{u\in\Gamma_{H_2}(u_2)} M_{H_2-u_2u}(x)) \\ &\quad -M_{H_1-u_1}(x)M_{H_2-u_2}(x), \end{aligned} \tag{2.6}$$

$$\begin{aligned} M_{G^*}(x) &= x^2M_{H_1-u_1}(x)M_{H_2-u_2}(x) - M_{H_1-u_1}(x)M_{H_2-u_2}(x) \\ &\quad -xM_{H_1-u_1}(x)\sum_{u\in\Gamma_{H_2}(u_2)} M_{H_2-u_2u}(x) \\ &\quad -xM_{H_2-u_2}(x)\sum_{u\in\Gamma_{H_1}(u_1)} M_{H_1-u_1u}(x). \end{aligned} \tag{2.7}$$

(2.6)-(2.7)

$$M_G(x) - M_{G^*}(x) = \sum_{u\in\Gamma_{H_2}(u_2)} M_{H_2-u_2u}(x) \sum_{u\in\Gamma_{H_1}(u_1)} M_{H_1-u_1u}(x). \tag{2.8}$$

In right hand side of equation (2.8) all graph $H_i - u_iu$, $i = 1, 2$ are subgraphs of G, By Lemma 2.3 and Corollary 2.7, for all $x \geq \theta(G)$, $M_{H_i-u_iu}(x) > 0$. Then $M_G(x) - M_{G^*}(x) > 0$. Hence

$$M(G) < M(G^*).$$

In particular, if e is an pendant edge of G then $G^* \cong G$, and

$$M(G^*) = M(G).$$

Now we prove that the coefficients of each matching polynomial satisfy

$$G \succ G^*, \quad e.g. \;\; m(G,k) \geq m(G^*).$$

From the structure of G and G^*, we have $m(G,k) = m(G^*,k)$ if a k-matching contains e both in graph G and G^*. Let us first consider a k-matching M of G.

Case 1. if $e \in M$, then

$$m(G,k) = m(G - \{u,v\}, k-1) = \sum_{i=0}^{k-1} m(H_1 - u_1, i)m(H_2 - u_2, k-1-i).$$

Case 2. If $e \notin M$, then $m(G,k) = \sum_{i=0}^{k} m(H_1,i)m(H_2,k-i)$. Hence, together we have

$$m(G,k) = \sum_{i=0}^{k-1} m(H_1-u_1,i)m(H_2-u_2,k-1-i) + \sum_{i=0}^{k} m(H_1,i)m(H_2,k-i). \quad (2.9)$$

Similarly, for G^* we have

$$m(G^*,k) = \sum_{i=0}^{k-1} m(H_1-u_1,i)m(H_2-u_2,k-1-i) + m(G \diamond e,k). \quad (2.10)$$

It is obviously that $m(G \diamond e,k) < \sum_{i=0}^{k} m(H_1,i)m(H_2,k-i)$. Therefore, Equation (2.9)-(2.10),

$$m(G,k) - m(G^*,k) > 0.$$

Lemma is proved. ∎

3 Main results of this paper

In this section we present the extremal graphs with respect to largest matching root, Hosoya index, and matching energy of graphs in $\mathscr{U}_n, \mathscr{B}_n$ and $\mathscr{T}_n$. Let n be sufficiently large that we can have a desired different kind of graphs. By using the Lammas obtained in Section 2, we characterize the extremal graphs in each kind of graphs. We begin with an Observation 3.1.

Observation 3.1 *Let $\alpha'(G)$ be the maximum size of matching. If*

$$\alpha'(G_1) \geq \alpha'(G_2),$$

then

$$m(G_1,k) \geq m(G_2,k),$$

for $0 \leq k \leq \min\{\alpha'(G_1), \alpha'(G_2)\}$.

For trees we take non-pendant edges and by applying the Lemma 2.9 and Lemma 2.10 on corresponding edges, we can easily prove the following results for the largest matching roots

$$2\cos(\pi/(n+1)) = \theta(P_n) \leq \theta(T) \leq \theta(K_{1,n-1}) = \sqrt{n-1}$$

and for Hosoya index,

$$n = Z(K_{1,n-1}) \leq T \leq Z(P_n) = f_{n+1},$$

and for matching energy

$$2\sqrt{n-1} = ME(K_{1,n-1}) < ME(T) < ME(P_n) = 2\sum_{i=1}^{n} |\cos(\pi/(n+1))|.$$

The following we focus on the matching properties of the unicyclic graphs, bicyclic graphs and tricyclic graphs.

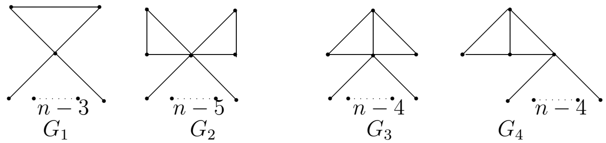

Fig. 3. Graphs in Theorem 3.2 and Theorem 3.3

For the matching energy of unicyclic graphs, Gutman and Wager (Theorem 6 [7]) obtain that $ME(S_n^+) \leq (ME(G)) \leq ME(C_n)$, as an application of our transformations, we present a proof and also give the bounds for each graph index among unicyclic graphs. In the Theorem 3.2, where $S_n^+ \cong G_1$.

Theorem 3.2 *[11] Let $\mathscr{U}_n$ be the unicyclic graphs. Then $G \in \mathscr{U}_n$, we have*

$$\theta(G) < \theta(G_1) = \sqrt{\frac{n + \sqrt{n^2 - 4(n-3)}}{2}}, \tag{3.1}$$

and the Hosoya index

$$Z(G) \geq Z(G_1) = 2n - 2, \tag{3.2}$$

and the matching energy $M(G) \geq M(G_1)$, and

$$ME(G_1) = 2[\sqrt{\frac{n - \sqrt{n^2 - 4(n-3)}}{2}} + \sqrt{\frac{n + \sqrt{n^2 - 4(n-3)}}{2}}]. \tag{3.3}$$

Proof. We take edges on the cycle (the length of cycle is great than three), and the edges which are not pendant edges, by using the transformations in Lemma 2.9 and Lemma 2.10. After finite times, we get the extremal graph with respect to largest matching root and Hosoya index, which is shown in Fig.3. G_1. The matching polynomial of G_1 is

$$M_{G_1}(x) = x^n - nx^{n-2} + (n-3)x^{n-4} = x^{n-4}(x^4 - nx^2 + n - 3).$$

By calculating the largest matching root, Hosoya index, and the matching energy, the proof is complete. ∎

Theorem 3.3 *Let $\mathscr{B}_n$ be the bicyclic graphs on n vertices. Then for any $G \in \mathscr{B}_n$, the following hold.*

$$\theta(G) < \theta(G_3) = \sqrt{\frac{n+1+\sqrt{(n+1)^2-8(n-3)}}{2}}, \tag{3.4}$$

and the Hosoya index

$$3n-4 = Z(G_3) \le Z(G), \tag{3.5}$$

and the matching energy $ME(G_3) \le ME(G)$, and

$$ME(G_3) = 2[\sqrt{\frac{n+1+\sqrt{n^2-6n+25}}{2}} + \sqrt{\frac{n+1-\sqrt{n^2-6n+25}}{2}}]. \tag{3.6}$$

Proof. We take the edges on the cycles (the length of cycles are greater than three) and non-pendant edges on the trees. By applying Lemma 2.9 and Lemma 2.10 finite times, we get the extremal graphs with respect to largest matching root, Hosoya index, matching energy, which are graphs G_2, G_3 and G_4 shown in Fig.3. It is easily see that the matching number of them satisfy

$$2 = \alpha'(G_3) = \alpha'(G_4) < \alpha'(G_2) = 3.$$

Hence, by Observation 3.1, the graph G_3 maximize the largest matching root and minimize the Hosoya index, and matching energy. By Lemma 2.1 and Lemma 2.2 we calculate the matching polynomial of G_2, G_3, G_4.

$$M_{G_2}(x) = x^n - (n+1)x^{n-2} + (2n-5)x^{n-4} - (n-5)x^{n-6}.$$

$$Z(G_2) = 4n-8,$$

and

$$M_{G_3}(x) = x^n - (n+1)x^{n-2} + 2(n-3)x^{n-4}.$$

$$Z(G_3) = 3n-4,$$

and the matching polynomial of G_4 is

$$M_{G_4}(x) = x^n - (n+1)x^{n-2} + (2n-10)x^{n-4}.$$

$$Z(G_4) = 4n-8.$$

Form above we saw that G_3 has the largest matching root and minimum Hosoya index.

$$\theta(G_3) = \sqrt{\frac{n+1+\sqrt{(n+1)^2-8(n-3)}}{2}}, Z(G_3) = 3n-4.$$

The minimum matching energy is

$$ME(G_3) = 2[\sqrt{\frac{n+1+\sqrt{(n+1)^2-8(n-3)}}{2}} + \sqrt{\frac{n+1-\sqrt{(n+1)^2-8(n-3)}}{2}}].$$

∎

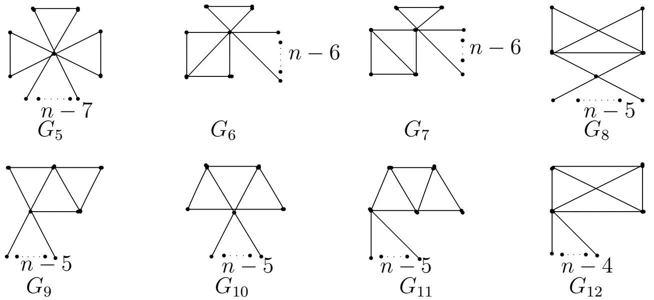

Fig.4. Graphs in Theorem 3.4

Theorem 3.4 *Let $\mathscr{T}_n$ be the set of tricyclic graphs. For any graph $G \in \mathscr{T}_n$, the largest matching root*

$$\theta(G) < \theta(G_{12}) = \sqrt{\frac{n+2+\sqrt{n^2-8n+40}}{2}}, \tag{3.7}$$

The minimum Hosoya index

$$Z(G) > Z(G_{12}) = 4n-6, \tag{3.8}$$

and the minimal matching energy, $ME(G) > ME(G_{12})$, and

$$ME(G_{12}) = 2[\sqrt{\frac{n+2+\sqrt{n^2-8n+40}}{2}} + \sqrt{\frac{n+2-\sqrt{n^2-8n+40}}{2}}]. \tag{3.9}$$

Where G_{12} is the graph in Fig.4.

Proof. For a tree $G \in \mathscr{T}_n$, we apply Lemma 2.9 and Lemma 2.10 on the edges of the cycles (the length of cycle is greater than three) and on non-pendant of trees. After finite times the graph which has the minimum matching number and the largest matching roots are the graphs shown in Fig.4. $\alpha'(G_5) = 4, \alpha'(G_6) = \ldots = \alpha'(G_{11}) = 3$, and $\alpha'(G_{12}) = \alpha'(G_{13}) = 2$. Hence, with Observation 3.1, graph G_{12} has the largest matching root and minimum Hosoya index and minimum matching energy. The matching polynomial of G_{12} is

$$M_{G_{12}}(x) = x^n - (n+2)x^{n-2} + 3(n-3)x^{n-4}.$$

The Hosoya index is

$$Z(G_{12}) = 4n - 6.$$

The largest matching root is a root of the following polynomial,

$$\theta(G_{12}) = \sqrt{\frac{n+2+\sqrt{(n+2)^2 - 12(n-3)}}{2}}.$$

The matching energy,

$$ME(G_5) = 2[\sqrt{\frac{n+2+\sqrt{n^2-8n+40}}{2}} + \sqrt{\frac{n+2-\sqrt{n^2-8n+40}}{2}}].$$

∎

Form the above discuss we find that for a connected graph, the graph has small Hosoya index and the graph will have larger largest matching root and has less matching energy.

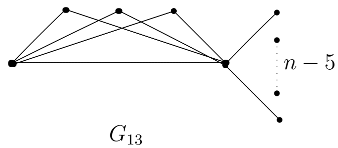

Fig. 4. Matching equivalent graph G_{13}

Graph G and H are *matching equivalent*, written as $G \sim H$ if $M_{G_1}(x) = M_{G_2}(x)$. In the following remark we point out that in $\mathscr{T}_n$, G_{12} has a matching equivalent graph G_{13}, also see in [15].

Remark 3.5 *There exists another graph G_{13} in $\mathscr{T}_n$ has minimum matching energy, furthermore they are matching equivalent, e.g. $G_{12} \sim G_{13}$.*

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