The bipartite unicyclic graphs with the first $\lfloor \frac{n-3}{4} \rfloor$ largest matching energies

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Abstract

The theory of matching energy of graphs since be proposed by Gutman and Wagner in 2012, has attracted more and more attention. Denote by $\mathcal{B}_{n,m}$ the class of bipartite graphs with order n and size m. In particular, $\mathcal{B}_{n,n}$ denotes the set of bipartite unicyclic graphs, which is an interesting class of graphs. In this paper, for odd n, we characterize the bipartite unicyclic graphs with the first $\lfloor \frac{n-3}{4} \rfloor$ largest matching energies. There is an interesting correspondence: we conclude that the graph with the second maximal matching energy in $\mathcal{B}_{n,n}$ for odd $n \geq 11$ is P_n^6, which is the only graph attaining the maximum value of the energy among all the (bipartite) unicyclic graphs for $n \geq 16$.

Keywords: matching energy; bipartite unicyclic graphs; quasi-order; Coulson integral formula

1. Introduction

In theoretical chemistry and biology, molecular structure descriptors are used for modeling physical-chemical, toxicologic, pharmacologic, biological and other properties of chemical compounds. These descriptors are mainly divided into three types: degree-based indices, distance-based indices and spectrum-based indices. Degree-based indices [64] contain (general) Randić index [52, 53], (general) zeroth order Randić index [40, 41], Zagreb index [1, 29, 38, 47, 59, 66, 68], connective eccentricity index [72] and so on. Distance-based indices [70] include the Balaban index [15], the Wiener index [20, 39, 48, 57, 58, 65] and Wiener polarity index [60], the Szeged index [3, 21], ABC index [63], the Kirchhoff index [50], the Harary index [5]. Eigenvalues of graphs, various of graph energies [7, 8, 9, 17, 16, 31, 61], HOMO-LUMO index [54, 62] belong to spectrum-based indices. Actually, there are also some topological indices defined based on both degrees and distances, such as degree distance [19], graph entropies [10].

In 1977, Gutman [23] proposed the concept of graph energy. The *energy* of a simple graph G is defined as the sum of the absolute values of its eigenvalues, namely,

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

where $\lambda_1, \lambda_2, \ldots, \lambda_n$ denote the eigenvalues of G. The graph energy has been rather widely studied by theoretical chemists and mathematicians. For details, we refer the book on graph energy [55] and some new recent references [42, 43, 56].

A *matching* in a graph G is a set of pairwise nonadjacent edges. A matching M is called a *k-matching* if the size of M is k. Let $m(G, k)$ denote the number of k-matchings of G, where $m(G, 1) = m$ 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

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

Similar to graph energy, in [37], Gutman and Wagner proposed the concept of matching energy. They defined the *matching energy* of a graph G as

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

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 ([37]). *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*

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

Formula (1) is called the *Coulson integral formula* of matching energy. Obviously, by the monotonicity of the logarithm function, this formula implies that the matching energy of a graph G is a monotonically increasing function of any $m(G,k)$. Particularly, if G_1 and G_2 are two graphs for which $m(G_1,k) \geq m(G_2,k)$ holds for all $k \geq 0$, then $ME(G_1) \geq ME(G_2)$. If, in addition, $m(G_1,k) > m(G_2,k)$ for at least one k, then $ME(G_1) > ME(G_2)$. Thus, we can define a *quasi-order* $\succeq$ as follows: If G_1 and G_2 are two graphs, then

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

And if $G_1 \succeq G_2$ we say that G_1 is *m-greater than* G_2 or G_2 is *m-smaller than* G_1, which is also denoted by $G_2 \preceq G_1$. If $G_1 \succeq G_2$ and $G_2 \succeq G_1$, the graphs G_1 and G_2 are said to be *m-equivalent*, denote it by $G_1 \sim G_2$. If $G_1 \succeq G_2$, but the graphs G_1 and G_2 are not m-equivalent (i.e., there exists some k such that $m(G_1,k) > m(G_2,k)$), then we say that G_1 is *strictly m-greater than* G_2, write $G_1 \succ G_2$. If neither $G_1 \succeq G_2$ nor $G_2 \succeq G_1$, the two graphs G_1 and G_2 are said to be *m-incomparable* and we denote this by $G_1 \# G_2$.

According to Eq.(1) and Eq.(2), we get $G_1 \succeq G_2 \Longrightarrow ME(G_1) \geq ME(G_2)$ and $G_1 \succ G_2 \Longrightarrow ME(G_1) > ME(G_2)$ directly.

In [37], 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 [33].

As the research of extremal energy is an amusing work, the study on extremal matching energy is also interesting. In [37], the authors gave some elementary results on the matching energy and obtained that $ME(S_n^+) \leq ME(G) \leq ME(C_n)$ for any unicyclic graph G of order n, where S_n^+ is the graph obtained by adding a new edge to the star S_n. In [46], Ji et al. characterized the graphs with the extremal matching energy among all bicyclic graphs, while Chen and Shi [11] proved the same extremal results for tricyclic graphs. In [12], Chen et al. characterized the graphs with minimal matching energy among all unicyclic and bicyclic graphs with a given diameter d. Some more extremal results on matching energy of graphs see [14, 51, 67, 69, 71].

All graphs considered here are simple, finite and undirected. We follow the book [6] for all the notations and terminology not defined here. By convention, denote by P_n, C_n, S_n the path, cycle, star of order n. $\mathcal{T}_n$ denotes the set of trees with n vertices. Referring to graphs with no odd cycles as *even-cycle graphs*, i.e., the bipartite graphs. Denote by $\mathcal{B}_n$ the class of even-cycle graphs with order n, and $\mathcal{B}_{n,m}$ the class of graphs in $\mathcal{B}_n$

with m edges. Especially, we call the graphs in $\mathcal{B}_{n,n}$ as *bipartite unicyclic graphs*, which is an interesting class of graphs. What's more, we introduce some new notations appeared in [37] and [49]. The *sun graph*, denoted by $C_l(P_{s_1+1}, \ldots, P_{s_l+1})$, is one obtained from the cycle $C_l = v_1v_2\ldots v_lv_1$ by identifying one pendent vertex of path P_{s_i+1} with vertex v_i for $i = 1, \ldots, l$. Note that $C_l(P_{n-l+1}, P_1 \ldots, P_1)$ is also called *lollipop graph* and abbreviated as P_n^l. Let G be a connected graph with at least two vertices, and let u be one of its vertices. Denote by $P(n, k, G, u)$ the graph obtained by identifying u with the vertex v_k of a simple path $P = v_1v_2\ldots v_n$. We in the following give the graphs $C_l(P_{s_1+1}, \ldots, P_{s_l+1})$ and $P(s, k, P^l_{n-s+1}, u)$ for examples, as shown in Fig 1.

In [13], the authors determined the graphs with the second through the fourth maximal matching energies in $\mathcal{O}_{n,n}$ when n is odd, where $\mathcal{O}_{n,n}$ is the set of unicyclic odd-cycle graphs. Inspired by this, we investigate the extremal values of matching energy of bipartite unicyclic graphs. We characterize in this paper the bipartite unicyclic graphs with the first $\lfloor \frac{n-3}{4} \rfloor$ largest matching energies when n is odd. One of the most interesting things is that the extremal graphs for matching energy in this paper are P_n^l for some values of l, which are related to the extremal graph (i.e., P_n^6) having maximal energy among all the bipartite unicyclic graphs for $n \geq 16$ (see [45]). In fact, when $n \geq 11$, with regard to matching energy, the graph P_n^6 is precisely the second maximal graph in $\mathcal{B}_{n,n}$ for n being odd.

2. Preliminaries

In this section, we list several known results at first. Then some useful lemmas are shown, which play the key roles in proving our main results.

Lemma 1 ([18, 25]). *Let G be a simple graph, $e = uv$ be an edge of G, and $N(u) = \{v_1(= v), v_2, \ldots, v_j\}$ be the set of all neighbors of u in G. Then we have*

$$m(G, k) = m(G - uv, k) + m(G - u - v, k - 1), \tag{3}$$

$$m(G, k) = m(G - u, k) + \sum_{i=1}^{j} m(G - u - v_i, k - 1). \tag{4}$$

From Lemma 1, we know that $m(P_1 \cup G, k) = m(G, k)$. And one can also obtain that

Lemma 2 ([12]). *Let G be a simple graph and H be a subgraph (resp. proper subgraph) of G. Then $G \succeq H$ (resp. $\succ H$).*

Lemma 3 ([30]). *Now H_1 and H_2 are two graphs. If $H_1 \succ H_2$, then $H_1 \cup G \succ H_2 \cup G$, where G is an arbitrary graph.*

Lemma 4 ([49]). *Let n, l be positive integers, $n > l \geq 3$. Denote by $\mathcal{U}_{l,n}$ the set of unicyclic graphs with n vertices and a cycle of length l, then for any graph $G \in \mathcal{U}_{l,n}$, we have*

$$ME(P_n^l) \geq ME(G),$$

with equality if and only if $G \cong P_n^l$.

Actually, the authors in [49] proved that $P_n^l \succ G$ for any $G \in \mathcal{U}_{l,n} \setminus \{P_n^l\}$.

Lemma 5 ([23, 46]). *In regard to the quasi-order $\succ$, we have the following ordering:*

$$P_n \succ P_2 \cup P_{n-2} \succ P_4 \cup P_{n-4} \succ \cdots \succ P_3 \cup P_{n-3} \succ P_1 \cup P_{n-1}.$$

Lemma 6 ([23, 37]). *If F is a forest with $n(n \geq 6)$ vertices, then $F \preceq P_n$, with $F \sim P_n$ if and only if $F \cong P_n$.*

Lemma 7 ([37]). *Let G be a connected graph with at least two vertices, and let u be one of its vertices. Denote by $P(n, k, G, u)$ the graph obtained by identifying u with the vertex v_k of a simple path $v_1, v_2, \ldots, v_n$. Write $n = 4p + i$, $i \in \{1, 2, 3, 4\}$, and $l = \lfloor (i-1)/2 \rfloor$. Then the inequalities*

$$\begin{aligned} &ME(P(n,2,G,u)) < ME(P(n,4,G,u)) < \cdots < ME(P(n,2p+2l,G,u)) \\ &< ME(P(n,2p+1,G,u)) < \cdots < ME(P(n,3,G,u)) < ME(P(n,1,G,u)) \end{aligned}$$

hold.

Lemma 8 ([37]). *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).*

Lemma 9. *Let n be odd and l be even with $4 \le l \le n-3$. Then $P_n^l \succ P_n^{l+2}$.*

Proof. For $0 \le k \le \frac{n-1}{2}$, by Eq.(3),

$$m(P_n^l, k) = m(P_n, k) + m(P_{l-2} \cup P_{n-l}, k-1),$$

$$m(P_n^{l+2}, k) = m(P_n, k) + m(P_l \cup P_{n-l-2}, k-1).$$

Since n is odd but l is even, then $l-2$ and l are even, while $n-l$ and $n-l-2$ are odd. Applying Lemma 5, we know $P_{l-2} \cup P_{n-l} \succ P_l \cup P_{n-l-2}$. This deduces that $P_n^l \succ P_n^{l+2}$. ∎

Remark 1. Through simple calculations, it's easy to derive $P_n^l \sim P_n^{n-l+2}$. Then by the conclusion above, we get $P_n^{n-l+2} \succ P_n^{n-l}$. Notice that both $n-l+2$ and $n-l$ are odd, hence this result is in accordance with Lemma 8 in [13];

Remark 2. Taking advantage of the lemma above, for n being odd, we obtain $P_n^4 \succ P_n^6 \succ P_n^8 \succ \ldots \succ P_n^{n-5} \succ P_n^{n-3} \succ P_n^{n-1}$ directly.

Lemma 10. *Let G_1 and G_2 be two vertex-disjoint graphs. Then*

$$\alpha(G_1 \cup G_2, x) = \alpha(G_1, x) \cdot \alpha(G_2, x).$$

Proof. Set $n_1 = |V(G_1)|$, $n_2 = |V(G_2)|$, with $n_1 + n_2 = n$. Then

$$\begin{aligned}
\alpha(G_1 \cup G_2, x) &= \sum_{k \ge 0} (-1)^k m(G_1 \cup G_2, k) x^{n-2k} \\
&= \sum_{k \ge 0} (-1)^k \Big(\sum_{j=0}^{k} m(G_1, j) m(G_2, k-j) \Big) x^{n-2k} \\
&= \Big[\sum_{j \ge 0} (-1)^j m(G_1, j) x^{n_1 - 2j} \Big] \\
&\quad \cdot \Big[\sum_{k-j \ge 0} (-1)^{k-j} m(G_2, k-j) x^{n_2 - 2(k-j)} \Big] \\
&= \alpha(G_1, x) \cdot \alpha(G_2, x).
\end{aligned}$$

The proof is thus completed. ∎

Let $G \ncong C_n$ be a connected graph in $\mathcal{B}_{n,n}$. Denote the unique cycle of G by C_l. We call each maximal tree outside C_l with one vertex attached to some vertex of C_l a *"branch"* of G, namely, any two branches of G have no common vertices. It is both consistent and convenient to define a vertex in C_l with no neighbor outside C_l also as a branch of G. Any branch with just one vertex is referred to as *trivial*. All other branches are *nontrivial*. If $G \ncong C_n$ is a graph in $\mathcal{B}_{n,n}$ with l branches outside the unique cycle C_l. The i-th branch has $s_i + 1$ ($s_i \geq 0$) vertices for $i = 1, \ldots, l$, where $s_1 + s_2 + \ldots + s_l = n - l$. Then according to Lemma 8, the matching energy of G increases when each of the branches becomes a path (unless G is already such a graph). Thus $ME(G) \leq ME(C_l(P_{s_1+1}, P_{s_2+1}, \ldots, P_{s_l+1}))$, with equality if and only if $G \cong C_l(P_{s_1+1}, P_{s_2+1}, \ldots, P_{s_l+1})$. In the following, we will show that $C_l(P_{s_1+1}, P_{s_2+1}, \ldots, P_{s_l+1}) \preceq C_l(P_{s_1+1}, P_{n-l-s_1+1}, P_1, \ldots, P_1)$.

Lemma 11. *The graphs* $C_l(P_{s_1+1}, P_{s_2+1}, \ldots, P_{s_l+1})$ *and* $C_l(P_{s_1+1}, P_{n-l-s_1+1}, P_1, \ldots, P_1)$ *are shown in Fig 1 and Fig 2, respectively. Where l is even with* $4 \leq l \leq n-2$, $1 \leq s_1 \leq n-l-1$. *Then* $C_l(P_{s_1+1}, P_{s_2+1}, \ldots, P_{s_l+1}) \preceq C_l(P_{s_1+1}, P_{n-l-s_1+1}, P_1, \ldots, P_1)$, *with* $C_l(P_{s_1+1}, P_{s_2+1}, \ldots, P_{s_l+1}) \sim C_l(P_{s_1+1}, P_{n-l-s_1+1}, P_1, \ldots, P_1)$ *if and only if* $C_l(P_{s_1+1}, P_{s_2+1}, \ldots, P_{s_l+1}) \cong C_l(P_{s_1+1}, P_{n-l-s_1+1}, P_1, \ldots, P_1)$.

Proof. For $0 \leq k \leq \lfloor \frac{n}{2} \rfloor$, by Lemmas 1, 4 and 6, we have

$$\begin{aligned}
& m(C_l(P_{s_1+1}, P_{s_2+1}, \ldots, P_{s_l+1}), k) \\
= \ & m(C_l(P_{s_1+1}, P_{s_2+1}, \ldots, P_{s_l+1}) - uv_1, k) \\
& + m(C_l(P_{s_1+1}, P_{s_2+1}, \ldots, P_{s_l+1}) - u - v_1, k-1) \\
\leq \ & m(P_{n-s_1}^l \cup P_{s_1}, k) + m(P_{n-s_1-1} \cup P_{s_1-1}, k-1) \\
= \ & m(C_l(P_{s_1+1}, P_{n-l-s_1+1}, P_1, \ldots, P_1) - xw, k) \\
& + m(C_l(P_{s_1+1}, P_{n-l-s_1+1}, P_1, \ldots, P_1) - x - w, k-1) \\
= \ & m(C_l(P_{s_1+1}, P_{n-l-s_1+1}, P_1, \ldots, P_1), k).
\end{aligned}$$

Which yields that $C_l(P_{s_1+1}, P_{s_2+1}, \ldots, P_{s_l+1}) \preceq C_l(P_{s_1+1}, P_{n-l-s_1+1}, P_1, \ldots, P_1)$. The equality holds for all k if and only if $C_l(P_{s_1+1}, P_{s_2+1}, \ldots, P_{s_l+1}) - uv_1 \cong P_{n-s_1}^l \cup P_{s_1}$, meanwhile $C_l(P_{s_1+1}, P_{s_2+1}, \ldots, P_{s_l+1}) - u - v_1 \cong P_{n-s_1-1} \cup P_{s_1-1}$. That is, if and only if $C_l(P_{s_1+1}, P_{s_2+1}, \ldots, P_{s_l+1}) \cong C_l(P_{s_1+1}, P_{n-l-s_1+1}, P_1, \ldots, P_1)$. ∎

As a special case of Lemma 11, for the graphs $C_l(P_{s+1}, \underbrace{P_1, \ldots, P_1}_{t}, P_{n-l-s+1}, P_1, \ldots, P_1)$, where l is even with $4 \leq l \leq n-2$, $1 \leq s \leq n-l-1$. Let the two 3-degree vertices be x and y, if the number of vertices in the unique cycle between x and y is t with $1 \leq t \leq \frac{l-2}{2}$ (as shown in Fig 2).

Then it follows immediately that $C_l(P_{s+1}, \underbrace{P_1, \dots, P_1}_{t}, P_{n-l-s+1}, P_1, \dots, P_1) \prec$ $C_l(P_{s+1}, P_{n-l-s+1}, P_1, \dots, P_1)$.

Lemma 12. *Let l be even with $4 \leq l \leq n-2$, s be an integer with $1 \leq s \leq n-l-1$. Then $C_l(P_{s+1}, P_{n-l-s+1}, P_1, \dots, P_1) \preceq C_l(P_{n-l-1}, P_3, P_1, \dots, P_1)$ (these two graphs are shown in Fig 3), with $C_l(P_{s+1}, P_{n-l-s+1}, P_1, \dots, P_1) \sim C_l(P_{n-l-1}, P_3, P_1, \dots, P_1)$ if and only if $s = n-l-2$ or $s = 2$.*

Proof. For $0 \leq k \leq \lfloor \frac{n}{2} \rfloor$, we have

$$\begin{aligned}
& m(C_l(P_{s+1}, P_{n-l-s+1}, P_1, \dots, P_1), k) \\
= \; & m(C_l(P_{s+1}, P_{n-l-s+1}, P_1, \dots, P_1) - xy, k) \\
& + m(C_l(P_{s+1}, P_{n-l-s+1}, P_1, \dots, P_1) - x - y, k-1) \\
= \; & m(P_n, k) + m(P_{l-2} \cup P_s \cup P_{n-l-s}, k-1), \\
& m(C_l(P_{n-l-1}, P_3, P_1, \dots, P_1), k) \\
= \; & m(C_l(P_{n-l-1}, P_3, P_1, \dots, P_1) - xy, k) \\
& + m(C_l(P_{n-l-1}, P_3, P_1, \dots, P_1) - x - y, k-1) \\
= \; & m(P_n, k) + m(P_{l-2} \cup P_{n-l-2} \cup P_2, k-1).
\end{aligned}$$

Since $P_s \cup P_{n-l-s} \preceq P_{n-l-2} \cup P_2$ by Lemma 5, then $m(P_{l-2} \cup P_s \cup P_{n-l-s}, k-1) \leq m(P_{l-2} \cup P_{n-l-2} \cup P_2, k-1)$, which yields that $m(C_l(P_{s+1}, P_{n-l-s+1}, P_1, \dots, P_1), k) \leq m(C_l(P_{n-l-1}, P_3, P_1, \dots, P_1), k)$. The equality holds for all k if and only if $P_s \cup P_{n-l-s} \cong P_{n-l-2} \cup P_2$, namely, $s = n-l-2$ or $s = 2$. Hence, the result holds. ∎

Lemma 13. *Let n be odd with $n \geq 9$, l be even with $4 \leq l \leq n-3$. Then $P(n-4, 3, P_5^4, u_1) \succ C_l(P_{n-l-1}, P_3, P_1, \dots, P_1)$. Where the graph $P(n-4, 3, P_5^4, u_1)$ is shown in Fig 4.*

Proof. For $0 \leq k \leq \frac{n-1}{2}$, Eq.(3) leads to

$$\begin{aligned}
& m(P(n-4, 3, P_5^4, u_1), k) \\
= \; & m(P(n-4, 3, P_5^4, u_1) - u_1 v_2, k) \\
& + m(P(n-4, 3, P_5^4, u_1) - u_1 - v_2, k-1) \\
= \; & m(P_2 \cup P_{n-2}^4, k) + m(C_4 \cup P_{n-7}, k-1) \\
= \; & m(P_2 \cup P_{n-2}^4, k) + m(P_4 \cup P_{n-7}, k-1) + m(P_2 \cup P_{n-7}, k-2),
\end{aligned}$$

$$\begin{aligned} & m(C_l(P_{n-l-1}, P_3, P_1, \ldots, P_1), k) \\ = \; & m(C_l(P_{n-l-1}, P_3, P_1, \ldots, P_1) - yw, k) \\ & + m(C_l(P_{n-l-1}, P_3, P_1, \ldots, P_1) - y - w, k-1) \\ = \; & m(P_2 \cup P^l_{n-2}, k) + m(P_{n-3}, k-1) \\ = \; & m(P_2 \cup P^l_{n-2}, k) + m(P_4 \cup P_{n-7}, k-1) + m(P_3 \cup P_{n-8}, k-2). \end{aligned}$$

Since n is odd with $n \geq 9$ and $4 \leq l \leq n-3$, then by Lemmas 3, 5 and Remark 2 after Lemma 9, we get $P_2 \cup P_{n-7} \succ P_3 \cup P_{n-8}$ and $P_2 \cup P^4_{n-2} \succeq P_2 \cup P^l_{n-2}$. Hence $m(P(n-4, 3, P^4_5, u_1), k) \geq m(C_l(P_{n-l-1}, P_3, P_1, \ldots, P_1), k)$. It follows from $P_2 \cup P_{n-7} \succ P_3 \cup P_{n-8}$ that there exists some k_0 such that $m(P_2 \cup P_{n-7}, k_0) > m(P_3 \cup P_{n-8}, k_0)$, which deduces $m(P(n-4, 3, P^4_5, u_1), k_0 + 2) > m(C_l(P_{n-l-1}, P_3, P_1, \ldots, P_1), k_0 + 2)$. Therefore, $P(n-4, 3, P^4_5, u_1) \succ C_l(P_{n-l-1}, P_3, P_1, \ldots, P_1)$. ∎

Summarizing the above analysis, the graphs in $\mathcal{B}_{n,n}$ with more than one nontrivial branch have been discussed. Now consider the graph G in $\mathcal{B}_{n,n}$ with just one nontrivial branch. This branch is connected to the unique cycle C_l of G by a cut vertex, say u_0. The $n-l$ vertices outside C_l are denoted by $u_1, u_2, \ldots, u_{n-l}$. Suppose $G \ncong P^l_n$. If $d(u_0) \geq 4$, then by Lemma 7 and Lemma 8, we know that $ME(G) \leq ME(P(n-l+1, 3, C_l, u_0))$, with equality if and only if $G \cong P(n-l+1, 3, C_l, u_0)$. If $d(u_0) = 3$, since $G \ncong P^l_n$, there exists some vertex in $\{u_1, u_2, \ldots, u_{n-l}\}$ having degree not less than 3. Assume that $d(u_i) \geq 3$ with $1 \leq i \leq n-l-2$, and $d(u_j) = 2$ for $1 \leq j \leq i-1$ (see Fig 4). Then similarly, we have $ME(G) \leq ME(P(n-l-i+1, 3, P^l_{l+i}, u_i))$, with equality if and only if $G \cong P(n-l-i+1, 3, P^l_{l+i}, u_i)$. The graphs $P(n-l+1, 3, C_l, u_0)$ and $P(n-l-i+1, 3, P^l_{l+i}, u_i)$ with $1 \leq i \leq n-l-3$ are shown in Fig 4.

Lemma 14. *Let n be odd with $n \geq 9$, l be even with $4 \leq l \leq n-3$. Then we can obtain $P(n-4, 3, P^4_5, u_1) \succ P(n-l+1, 3, C_l, u_0)$.*

Proof. For $0 \leq k \leq \frac{n-1}{2}$, one can check that

$$\begin{aligned} & m(P(n-4, 3, P^4_5, u_1), k) \\ = \; & m(P(n-4, 3, P^4_5, u_1) - u_1 v_2, k) \\ & + m(P(n-4, 3, P^4_5, u_1) - u_1 - v_2, k-1) \\ = \; & m(P_2 \cup P^4_{n-2}, k) + m(C_4 \cup P_{n-7}, k-1) \\ \geq \; & m(P_2 \cup P^4_{n-2}, k) + m(P_4 \cup P_{n-7}, k-1), \end{aligned}$$

$$
\begin{aligned}
& m(P(n-l+1,3,C_l,u_0),k) \\
= \;& m(P(n-l+1,3,C_l,u_0)-u_0v_2,k) \\
& +m(P(n-l+1,3,C_l,u_0)-u_0-v_2,k-1) \\
= \;& m(P_2\cup P_{n-2}^l,k)+m(P_{l-1}\cup P_{n-l-2},k-1).
\end{aligned}
$$

Since n is odd with $n\geq 9$ and l is even with $4\leq l\leq n-3$, then $P_4\cup P_{n-7}\succ P_{l-1}\cup P_{n-l-2}$ and $P_2\cup P_{n-2}^4\succeq P_2\cup P_{n-2}^l$. Hence $m(P(n-4,3,P_5^4,u_1),k)\geq m(P(n-l+1,3,C_l,u_0),k)$. Moreover, $m(P(n-4,3,P_5^4,u_1),2)>m(P(n-l+1,3,C_l,u_0),2)$. Hence $P(n-4,3,P_5^4,u_1)\succ P(n-l+1,3,C_l,u_0)$. ∎

Lemma 15. *Let n be odd, l be even with $4\leq l\leq n-5$, $2\leq i\leq n-l-3$. Then $P(n-l-i+1,3,P_{l+i}^l,u_i)\preceq P(5,3,P_{n-4}^l,u_{n-l-4})$, with $P(n-l-i+1,3,P_{l+i}^l,u_i)\sim P(5,3,P_{n-4}^l,u_{n-l-4})$ if and only if $P(n-l-i+1,3,P_{l+i}^l,u_i)\cong P(5,3,P_{n-4}^l,u_{n-l-4})$ (i.e., $i=n-l-4$). Where the graph $P(5,3,P_{n-4}^l,u_{n-l-4})$ is shown in Fig 5.*

Proof. For $0\leq k\leq \frac{n-1}{2}$,

$$
\begin{aligned}
& m(P(n-l-i+1,3,P_{l+i}^l,u_i),k) \\
= \;& m(P(n-l-i+1,3,P_{l+i}^l,u_i)-v_2u_i,k) \\
& +m(P(n-l-i+1,3,P_{l+i}^l,u_i)-v_2-u_i,k-1) \\
= \;& m(P_{n-2}^l\cup P_2,k)+m(P_{l+i-1}^l\cup P_{n-l-i-2},k-1) \\
= \;& m(P_{n-2}^l\cup P_2,k)+m(P_{l+i-1}\cup P_{n-l-i-2},k-1) \\
& +m(P_{l-2}\cup P_{i-1}\cup P_{n-l-i-2},k-2), \\
& m(P(5,3,P_{n-4}^l,u_{n-l-4}),k) \\
= \;& m(P(5,3,P_{n-4}^l,u_{n-l-4})-v_2u_{n-l-4},k) \\
& +m(P(5,3,P_{n-4}^l,u_{n-l-4})-v_2-u_{n-l-4},k-1) \\
= \;& m(P_{n-2}^l\cup P_2,k)+m(P_{n-5}^l\cup P_2,k-1) \\
= \;& m(P_{n-2}^l\cup P_2,k)+m(P_{n-5}\cup P_2,k-1) \\
& +m(P_{l-2}\cup P_{n-l-5}\cup P_2,k-2).
\end{aligned}
$$

Since $2\leq i\leq n-l-3$, then $P_{l+i-1}\cup P_{n-l-i-2}\preceq P_{n-5}\cup P_2$ and also $P_{l-2}\cup P_{i-1}\cup P_{n-l-i-2}\preceq P_{l-2}\cup P_{n-l-5}\cup P_2$. Which mean $m(P(n-l-i+1,3,P_{l+i}^l,u_i),k)\leq m(P(5,3,P_{n-4}^l,u_{n-l-4}),k)$. The equality holds for all k if and only if $i=n-l-4$. It follows that the proof is completed. ∎

Furthermore, if $i = n-l-2$ and $G \ncong P_n^l$, then $G \cong P(3,2,P_{n-2}^l,u_{n-l-2})$ (as shown in Fig 5). In this case, we can also arrive at $P(3,2,P_{n-2}^l,u_{n-l-2}) \prec P(5,3,P_{n-4}^l,u_{n-l-4})$.

Lemma 16. *For even l with $4 \le l \le n-5$, we have $P(3,2,P_{n-2}^l,u_{n-l-2}) \prec P(5,3,P_{n-4}^l,u_{n-l-4})$.*

Proof. For all $0 \le k \le \lfloor \frac{n}{2} \rfloor$, since $4 \le l \le n-5$,

$$\begin{aligned}
& m(P(3,2,P_{n-2}^l,u_{n-l-2}),k) \\
= \; & m(P(3,2,P_{n-2}^l,u_{n-l-2}) - u_{n-l-3}u_{n-l-2},k) \\
& + m(P(3,2,P_{n-2}^l,u_{n-l-2}) - u_{n-l-3} - u_{n-l-2},k-1) \\
= \; & m(P_{n-3}^l \cup P_3,k) + m(P_{n-4}^l,k-1) \\
= \; & m(P_{n-3} \cup P_3,k) + m(P_{l-2} \cup P_{n-l-3} \cup P_3,k-1) \\
& + m(P_{n-4},k-1) + m(P_{l-2} \cup P_{n-l-4},k-2), \\
& m(P(5,3,P_{n-4}^l,u_{n-l-4}),k) \\
= \; & m(P(5,3,P_{n-4}^l,u_{n-l-4}) - v_2u_{n-l-4},k) \\
& + m(P(5,3,P_{n-4}^l,u_{n-l-4}) - v_2 - u_{n-l-4},k-1) \\
= \; & m(P_{n-2}^l \cup P_2,k) + m(P_{n-5}^l \cup P_2,k-1) \\
= \; & m(P_{n-2} \cup P_2,k) + m(P_{l-2} \cup P_{n-l-2} \cup P_2,k-1) \\
& + m(P_{n-5} \cup P_2,k-1) + m(P_{l-2} \cup P_{n-l-5} \cup P_2,k-2).
\end{aligned}$$

Clearly, $P_{n-3} \cup P_3 \prec P_{n-2} \cup P_2$, $P_{l-2} \cup P_{n-l-3} \cup P_3 \preceq P_{l-2} \cup P_{n-l-2} \cup P_2$, $P_{n-4} \prec P_{n-5} \cup P_2$ and $P_{l-2} \cup P_{n-l-4} \preceq P_{l-2} \cup P_{n-l-5} \cup P_2$. Which imply that $P(3,2,P_{n-2}^l,u_{n-l-2}) \prec P(5,3,P_{n-4}^l,u_{n-l-4})$. ∎

Lemma 17. *Let $n \ge 13$ be odd, l be even with $6 \le l \le n-7$, then $P(5,3,P_{n-4}^4,u_{n-8}) \succ P(5,3,P_{n-4}^l,u_{n-l-4})$. Where the graph $P(5,3,P_{n-4}^4,u_{n-8})$ is shown in Fig 6.*

Proof. Since l is even and $6 \le l \le n-7$, then by Lemma 5, we have $P_2 \cup P_{n-6} \succ P_{l-2} \cup P_{n-l-2}$, $P_2 \cup P_{n-9} \succeq P_{l-2} \cup P_{n-l-5}$. For $k \ge 0$, by Lemma 1, we can obtain that

$$\begin{aligned}
& m(P(5,3,P_{n-4}^4,u_{n-8}),k) \\
= \; & m(P(5,3,P_{n-4}^4,u_{n-8}) - u_0w,k) \\
& + m(P(5,3,P_{n-4}^4,u_{n-8}) - u_0 - w,k-1)
\end{aligned}$$

$$
\begin{aligned}
&= m(P(5,3,P^4_{n-4},u_{n-8})-u_0w,k)\\
&\quad +m(P(5,3,P^4_{n-4},u_{n-8})-u_0-w-u_{n-8}v_2,k-1)\\
&\quad +m(P(5,3,P^4_{n-4},u_{n-8})-u_0-w-u_{n-8}-v_2,k-2)\\
&= m(P(5,3,P^4_{n-4},u_{n-8})-u_0w,k)+m(P_2\cup P_2\cup P_{n-6},k-1)\\
&\quad +m(P_2\cup P_2\cup P_{n-9},k-2)\\
&\geq m(P(5,3,P^l_{n-4},u_{n-l-4})-u_0w,k)+m(P_2\cup P_{l-2}\cup P_{n-l-2},k-1)\\
&\quad +m(P_2\cup P_{l-2}\cup P_{n-l-5},k-2)\\
&= m(P(5,3,P^l_{n-4},u_{n-l-4}),k).
\end{aligned}
$$

Since $P_2\cup P_{n-6}\succ P_{l-2}\cup P_{n-l-2}$, by Lemma 3, $P_2\cup P_2\cup P_{n-6}\succ P_2\cup P_{l-2}\cup P_{n-l-2}$. Thus there exists some k_0 such that $m(P_2\cup P_2\cup P_{n-6},k_0)>m(P_2\cup P_{l-2}\cup P_{n-l-2},k_0)$. So $m(P(5,3,P^4_{n-4},u_{n-8}),k_0+1)>m(P(5,3,P^l_{n-4},u_{n-l-4}),k_0+1)$. Therefore, $P(5,3,P^4_{n-4},u_{n-8})\succ P(5,3,P^l_{n-4},u_{n-l-4})$. ∎

Lemma 18. *Let n be odd with $n\geq 11$, then we have $P(n-4,3,P^4_5,u_1)\succ P(5,3,P^4_{n-4},u_{n-8})$.*

Proof. For all $k\geq 0$, applying Lemma 1, one can get

$$
\begin{aligned}
& m(P(n-4,3,P^4_5,u_1),k)\\
&= m(P(n-4,3,P^4_5,u_1)-u_1v_2,k)\\
&\quad +m(P(n-4,3,P^4_5,u_1)-u_1-v_2,k-1)\\
&= m(P_2\cup P^4_{n-2},k)+m(P(n-4,3,P^4_5,u_1)-u_1-v_2-u_3u_4,k-1)\\
&\quad +m(P(n-4,3,P^4_5,u_1)-u_1-v_2-u_3-u_4,k-2)\\
&= m(P_2\cup P^4_{n-2},k)+m(C_4\cup P_2\cup P_{n-9},k-1)+m(C_4\cup P_{n-10},k-2),\\
& m(P(5,3,P^4_{n-4},u_{n-8}),k)\\
&= m(P(5,3,P^4_{n-4},u_{n-8})-u_{n-8}v_2,k)\\
&\quad +m(P(5,3,P^4_{n-4},u_{n-8})-u_{n-8}-v_2,k-1)\\
&= m(P_2\cup P^4_{n-2},k)+m(P(5,3,P^4_{n-4},u_{n-8})-u_{n-8}-v_2-u_0u_1,k-1)\\
&\quad +m(P(5,3,P^4_{n-4},u_{n-8})-u_{n-8}-v_2-u_0-u_1,k-2)\\
&= m(P_2\cup P^4_{n-2},k)+m(C_4\cup P_2\cup P_{n-9},k-1)+m(P_2\cup P_3\cup P_{n-10},k-2).
\end{aligned}
$$

Obviously, $C_4\succ P_2\cup P_3$, by Lemma 3, we get $C_4\cup P_{n-10}\succ P_2\cup P_3\cup P_{n-10}$. Thus $m(C_4\cup P_{n-10},k-2)\geq m(P_2\cup P_3\cup P_{n-10},k-2)$, and then $m(P(n-4,3,P^4_5,u_1),k)\geq m(P(5,3,P^4_{n-4},u_{n-8}),k)$. Moreover, $m(P(n-4,3,P^4_5,u_1),3)>m(P(5,3,P^4_{n-4},u_{n-8}),3)$. Hence $P(n-4,3,P^4_5,u_1)\succ P(5,3,P^4_{n-4},u_{n-8})$. The proof is finished. ∎

Lemma 19. *Let $n \geq 13$ be odd, l be even with $6 \leq l \leq n-7$, then $P(n-4, 3, P_5^4, u_1) \succ P(n-l, 3, P_{l+1}^l, u_1)$. Where the graph $P(n-l, 3, P_{l+1}^l, u_1)$ is shown in Fig 6.*

Proof. For all $k \geq 0$, it follows from Lemma 1 that

$$\begin{aligned}
& m(P(n-4,3,P_5^4,u_1),k) \\
= \; & m(P(n-4,3,P_5^4,u_1)-u_0w,k)+m(P(n-4,3,P_5^4,u_1)-u_0-w,k-1) \\
= \; & m(P(n-4,3,P_5^4,u_1)-u_0w-u_1v_2,k) \\
& +m(P(n-4,3,P_5^4,u_1)-u_0w-u_1-v_2,k-1)+m(P_2\cup P_{n-4},k-1) \\
= \; & m(P_2\cup P_{n-2},k)+m(P_4\cup P_{n-7},k-1)+m(P_2\cup P_{n-4},k-1), \\
& m(P(n-l,3,P_{l+1}^l,u_1),k) \\
= \; & m(P(n-l,3,P_{l+1}^l,u_1)-u_0w,k) \\
& +m(P(n-l,3,P_{l+1}^l,u_1)-u_0-w,k-1) \\
= \; & m(P(n-l,3,P_{l+1}^l,u_1)-u_0w-u_1v_2,k) \\
& +m(P(n-l,3,P_{l+1}^l,u_1)-u_0w-u_1-v_2,k-1)+m(P_{l-2}\cup P_{n-l},k-1) \\
= \; & m(P_2\cup P_{n-2},k)+m(P_l\cup P_{n-l-3},k-1)+m(P_{l-2}\cup P_{n-l},k-1).
\end{aligned}$$

Since l is even and $6 \leq l \leq n-7$, then $P_4 \cup P_{n-7} \succeq P_l \cup P_{n-l-3}$, $P_2 \cup P_{n-4} \succ P_{l-2} \cup P_{n-l}$. Hence $m(P(n-4,3,P_5^4,u_1),k) \geq m(P(n-l,3,P_{l+1}^l,u_1),k)$. In particular, there exists some k_0 such that $m(P_2 \cup P_{n-4}, k_0) > m(P_{l-2} \cup P_{n-l}, k_0)$, which implies that $m(P(n-4,3,P_5^4,u_1),k_0+1) > m(P(n-l,3,P_{l+1}^l, u_1),k_0+1)$. Consequently, $P(n-4,3,P_5^4,u_1) \succ P(n-l,3,P_{l+1}^l,u_1)$. ∎

So far, what remaining to discuss is the comparing of $ME(P(n-4,3,P_5^4,u_1))$ and $ME(P_n^l)$. By utilizing the Coulson integral formula of matching energy, as well as the help of computer, we will show $ME(P(n-4,3,P_5^4,u_1)) < ME(P_n^l)$ for $4 \leq l \leq \frac{n+1}{2}$ in the next section.

3. Main results

Let G be a simple graph, e be an edge of G connecting the vertices v_r and v_s. By $G(e/j)$ we denote the graph obtained by inserting $j (j \geq 0)$ new vertices (of degree two) on the edge e. On the number of k-matchings of the graph $G(e/j)$, the property that $m(G(e/j+2),k) = m(G(e/j+1),k) + m(G(e/j),k-1)$ for all $j \geq 0$ was given in [30]. In addition, on the matching polynomial of $G(e/j)$, we have shown that $\alpha(G(e/j+2),x) = x\alpha(G(e/j+1),x) - \alpha(G(e/j),x)$ in [11].

Lemma 20. *For $3 \le l \le n-1$, the matching polynomials of P_n and P_n^l have the following forms:*

$$\alpha(P_n, x) = A_1(x)(Y_1(x))^n + A_2(x)(Y_2(x))^n;$$
$$\alpha(P_n^l, x) = B_1(x)(Y_1(x))^n + B_2(x)(Y_2(x))^n.$$

Where $Y_1(x) = \frac{x+\sqrt{x^2-4}}{2}$, $Y_2(x) = \frac{x-\sqrt{x^2-4}}{2}$.

Proof. By the definition of $G(e/j)$, $P_n = P_2(e_1/n-2)$ and $P_n^l = P_{n-l+3}^3(e_2/l-3)$, where e_1 is the unique edge of P_2, e_2 is one of the edges of the triangle in P_{n-l+3}^3. Hence both $\alpha(P_n, x)$ and $\alpha(P_n^l, x)$ satisfy the recursive formula

$$f(n, x) = xf(n-1, x) - f(n-2, x).$$

The general solution of this linear homogeneous recurrence relation is

$$f(n, x) = C_1(x)(Y_1(x))^n + C_2(x)(Y_2(x))^n,$$

where $Y_1(x) = \frac{x+\sqrt{x^2-4}}{2}$, $Y_2(x) = \frac{x-\sqrt{x^2-4}}{2}$, with $Y_1(x) + Y_2(x) = x$ and $Y_1(x)Y_2(x) = 1$. Take the initial values as $\alpha(P_2, x) = x^2 - 1$ and $\alpha(P_3, x) = x^3 - 2x$. We then get

$$\alpha(P_n, x) = A_1(x)(Y_1(x))^n + A_2(x)(Y_2(x))^n,$$

where $A_1(x) = \frac{Y_1(x)\alpha(P_3,x)-\alpha(P_2,x)}{(Y_1(x))^4-(Y_1(x))^2}$, $A_2(x) = \frac{Y_2(x)\alpha(P_3,x)-\alpha(P_2,x)}{(Y_2(x))^4-(Y_2(x))^2}$.

For $3 \le l \le n-1$, $m(P_n^l, k) = m(P_n, k) + m(P_{l-2} \cup P_{n-l}, k-1)$. So

$$\begin{aligned}
\alpha(P_n^l, x) &= \sum_{k\ge 0}(-1)^k m(P_n^l, k)x^{n-2k} \\
&= \sum_{k\ge 0}(-1)^k \Big(m(P_n, k) + m(P_{l-2} \cup P_{n-l}, k-1)\Big)x^{n-2k} \\
&= \sum_{k\ge 0}(-1)^k m(P_n, k)x^{n-2k} + \sum_{k\ge 0}(-1)^k m(P_{l-2} \cup P_{n-l}, k-1)x^{n-2k} \\
&= \alpha(P_n, x) - \alpha(P_{l-2} \cup P_{n-l}, x) \\
&= \alpha(P_n, x) - \alpha(P_{l-2}, x) \cdot \alpha(P_{n-l}, x) \\
&= A_1(x)(Y_1(x))^n + A_2(x)(Y_2(x))^n - \Big(A_1(x)(Y_1(x))^{l-2} + \\
&\quad A_2(x)(Y_2(x))^{l-2}\Big) \cdot \Big(A_1(x)(Y_1(x))^{n-l} + A_2(x)(Y_2(x))^{n-l}\Big) \\
&= A_1(x)(Y_1(x))^n - (A_1(x))^2(Y_1(x))^{n-2} \\
&\quad -A_1(x)A_2(x)(Y_1(x))^{l-2}(Y_2(x))^{n-l} + A_2(x)(Y_2(x))^n \\
&\quad -(A_2(x))^2(Y_2(x))^{n-2} - A_1(x)A_2(x)(Y_1(x))^{n-l}(Y_2(x))^{l-2}.
\end{aligned}$$

Therefore, $\alpha(P_n^l, x) = B_1(x)(Y_1(x))^n + B_2(x)(Y_2(x))^n$. Where

$$B_1(x) = A_1(x) - (A_1(x))^2(Y_2(x))^2 - A_1(x)A_2(x)(Y_2(x))^{2l-2},$$

$$B_2(x) = A_2(x) - (A_2(x))^2(Y_1(x))^2 - A_1(x)A_2(x)(Y_1(x))^{2l-2}$$

for $3 \leq l \leq \frac{n+2}{2}$;

$$B_1(x) = A_1(x) - (A_1(x))^2(Y_2(x))^2 - A_1(x)A_2(x)(Y_2(x))^{2n-2l+2},$$

$$B_2(x) = A_2(x) - (A_2(x))^2(Y_1(x))^2 - A_1(x)A_2(x)(Y_1(x))^{2n-2l+2}$$

for $\frac{n+2}{2} < l \leq n-1$.

We complete the proof. ∎

Lemma 21. *Let $n (n \geq 9)$ be odd and $4 \leq l \leq \frac{n+1}{2}$ be even. Then $ME(P(n-4, 3, P_5^4, u_1)) < ME(P_n^l)$.*

Proof. If $l = 4$, then by Lemma 4, we get $ME(P(n-4, 3, P_5^4, u_1)) < ME(P_n^4)$ directly. If $n = 9$, then $l = 4$, this is the case just discussed. Hence in the following we assume that $n \geq 11$ and $l \geq 6$. Obviously, $P(n-4, 3, P_5^4, u_1) = P(4, 3, P_5^4, u_1)(e/n-8)$, where e is the pendent edge incident with u_1 in $P(4, 3, P_5^4, u_1)$. Similarly,

$$\alpha(P(n-4, 3, P_5^4, u_1), x) = C_1(x)(Y_1(x))^n + C_2(x)(Y_2(x))^n$$

with $Y_1(x) = \frac{x+\sqrt{x^2-4}}{2}$, $Y_2(x) = \frac{x-\sqrt{x^2-4}}{2}$. The initial values can be chosen as:

$$\begin{aligned} \alpha(P(4, 3, P_5^4, u_1), x) &= C_1(x)(Y_1(x))^8 + C_2(x)(Y_2(x))^8 \\ &= x^8 - 8x^6 + 18x^4 - 12x^2 + 2; \\ \alpha(P(5, 3, P_5^4, u_1), x) &= C_1(x)(Y_1(x))^9 + C_2(x)(Y_2(x))^9 \\ &= x^9 - 9x^7 + 25x^5 - 25x^3 + 8x. \end{aligned}$$

Solving the above two equations, we get

$$C_1(x) = \frac{Y_1(x)\alpha(P(5, 3, P_5^4, u_1), x) - \alpha(P(4, 3, P_5^4, u_1), x)}{(Y_1(x))^{10} - (Y_1(x))^8},$$

$$C_2(x) = \frac{Y_2(x)\alpha(P(5, 3, P_5^4, u_1), x) - \alpha(P(4, 3, P_5^4, u_1), x)}{(Y_2(x))^{10} - (Y_2(x))^8}.$$

Set $Z_1(x) = -iY_1(ix) = \frac{x+\sqrt{x^2+4}}{2}$, $Z_2(x) = -iY_2(ix) = \frac{x-\sqrt{x^2+4}}{2}$, where $i^2 = -1$. Then we have $Y_1(ix) = iZ_1(x)$, $Y_2(ix) = iZ_2(x)$, $Z_1(x) \cdot Z_2(x) = -1$, $Z_1(x) + Z_2(x) = x$, $Z_1(x) - Z_2(x) = \sqrt{x^2+4}$. Besides, set

$$f_1 = -\alpha(P_2, ix) = x^2 + 1;$$

$$f_2 = i\alpha(P_3, ix) = x^3 + 2x;$$

$$g_1 = \alpha(P(4, 3, P_5^4, u_1), ix) = x^8 + 8x^6 + 18x^4 + 12x^2 + 2;$$

$$g_2 = -i\alpha(P(5, 3, P_5^4, u_1), ix) = x^9 + 9x^7 + 25x^5 + 25x^3 + 8x.$$

For $4 \leq l \leq \frac{n+1}{2}$, according to Lemma 20 as well as the results got above,

$$A_1(ix) = \frac{Y_1(ix)\alpha(P_3, ix) - \alpha(P_2, ix)}{(Y_1(ix))^4 - (Y_1(ix))^2} = \frac{Z_1(x)f_2 + f_1}{(Z_1(x))^4 + (Z_1(x))^2};$$

$$A_2(ix) = \frac{Y_2(ix)\alpha(P_3, ix) - \alpha(P_2, ix)}{(Y_2(ix))^4 - (Y_2(ix))^2} = \frac{Z_2(x)f_2 + f_1}{(Z_2(x))^4 + (Z_2(x))^2};$$

$$\begin{aligned}
B_1(ix) &= A_1(ix) - (A_1(ix))^2(Y_2(ix))^2 - A_1(ix)A_2(ix)(Y_2(ix))^{2l-2} \\
&= \frac{Z_1(x)f_2 + f_1}{(Z_1(x))^4 + (Z_1(x))^2} + \frac{(Z_1(x)f_2 + f_1)^2}{(Z_1(x))^2((Z_1(x))^4 + (Z_1(x))^2)^2} \\
&\quad + \frac{(Z_1(x)f_2 + f_1)(Z_2(x)f_2 + f_1)(Z_2(x))^{2l-2}}{((Z_1(x))^4 + (Z_1(x))^2)((Z_2(x))^4 + (Z_2(x))^2)}; \\
B_2(ix) &= A_2(ix) - (A_2(ix))^2(Y_1(ix))^2 - A_1(ix)A_2(ix)(Y_1(ix))^{2l-2} \\
&= \frac{Z_2(x)f_2 + f_1}{(Z_2(x))^4 + (Z_2(x))^2} + \frac{(Z_2(x)f_2 + f_1)^2}{(Z_2(x))^2((Z_2(x))^4 + (Z_2(x))^2)^2} \\
&\quad + \frac{(Z_1(x)f_2 + f_1)(Z_2(x)f_2 + f_1)(Z_1(x))^{2l-2}}{((Z_1(x))^4 + (Z_1(x))^2)((Z_2(x))^4 + (Z_2(x))^2)}; \\
C_1(ix) &= \frac{Y_1(ix)\alpha(P(5, 3, P_5^4, u_1), ix) - \alpha(P(4, 3, P_5^4, u_1), ix)}{(Y_1(ix))^{10} - (Y_1(ix))^8} \\
&= \frac{Z_1(x)g_2 + g_1}{(Z_1(x))^{10} + (Z_1(x))^8}; \\
C_2(ix) &= \frac{Y_2(ix)\alpha(P(5, 3, P_5^4, u_1), ix) - \alpha(P(4, 3, P_5^4, u_1), ix)}{(Y_2(ix))^{10} - (Y_2(ix))^8} \\
&= \frac{Z_2(x)g_2 + g_1}{(Z_2(x))^{10} + (Z_2(x))^8}.
\end{aligned}$$

And then

$$\begin{aligned}
& ME(P(n-4,3,P_5^4,u_1)) - ME(P_n^l) \\
= & \frac{2}{\pi}\int_0^\infty \frac{1}{x^2}\ln\Big[\sum_{k\geq 0} m(P(n-4,3,P_5^4,u_1),k)x^{2k}\Big]dx \\
& -\frac{2}{\pi}\int_0^\infty \frac{1}{x^2}\ln\Big[\sum_{k\geq 0} m(P_n^l,k)x^{2k}\Big]dx \\
= & \frac{2}{\pi}\int_0^\infty \ln\frac{\alpha(P(n-4,3,P_5^4,u_1),ix)}{\alpha(P_n^l,ix)}dx \\
= & \frac{2}{\pi}\int_0^\infty \ln\frac{C_1(ix)(Y_1(ix))^n + C_2(ix)(Y_2(ix))^n}{B_1(ix)(Y_1(ix))^n + B_2(ix)(Y_2(ix))^n}dx.
\end{aligned}$$

Since n is odd,

$$\ln\frac{C_1(ix)(Y_1(ix))^{n+2} + C_2(ix)(Y_2(ix))^{n+2}}{B_1(ix)(Y_1(ix))^{n+2} + B_2(ix)(Y_2(ix))^{n+2}} - \ln\frac{C_1(ix)(Y_1(ix))^n + C_2(ix)(Y_2(ix))^n}{B_1(ix)(Y_1(ix))^n + B_2(ix)(Y_2(ix))^n}$$

$$= \ln\Big(1 + \frac{K_0(x)}{H_0(n,x)}\Big).$$

Where

$$\begin{aligned}
K_0(x) &= \Big(C_1(ix)(Y_1(ix))^{n+2} + C_2(ix)(Y_2(ix))^{n+2}\Big) \\
&\quad \cdot\Big(B_1(ix)(Y_1(ix))^n + B_2(ix)(Y_2(ix))^n\Big) \\
&\quad -\Big(B_1(ix)(Y_1(ix))^{n+2} + B_2(ix)(Y_2(ix))^{n+2}\Big) \\
&\quad \cdot\Big(C_1(ix)(Y_1(ix))^n + C_2(ix)(Y_2(ix))^n\Big) \\
&= \Big(C_1(ix)B_2(ix) - C_2(ix)B_1(ix)\Big)\Big((Y_1(ix))^2 - (Y_2(ix))^2\Big) \\
&= \Big(C_1(ix)B_2(ix) - C_2(ix)B_1(ix)\Big)\Big(-x\sqrt{x^2+4}\Big); \\
H_0(n,x) &= \Big(B_1(ix)(Y_1(ix))^{n+2} + B_2(ix)(Y_2(ix))^{n+2}\Big) \\
&\quad \cdot\Big(C_1(ix)(Y_1(ix))^n + C_2(ix)(Y_2(ix))^n\Big) \\
&= \alpha(P_{n+2}^l, ix)\cdot\alpha(P(n-4,3,P_5^4,u_1),ix) \\
&= \Big(i^{n+2}\sum_{k\geq 0} m(P_{n+2}^l,k)x^{n+2-2k}\Big)
\end{aligned}$$

$$
\begin{aligned}
&\cdot\Big(i^n\sum_{k\geq 0} m(P(n-4,3,P_5^4,u_1),k)x^{n-2k}\Big)\\
= \;& i^{2n+2}\Big(\sum_{k\geq 0} m(P_{n+2}^l,k)x^{n+2-2k}\Big)\\
&\cdot\Big(\sum_{k\geq 0} m(P(n-4,3,P_5^4,u_1),k)x^{n-2k}\Big)\\
= \;& \Big(\sum_{k\geq 0} m(P_{n+2}^l,k)x^{n+2-2k}\Big)\Big(\sum_{k\geq 0} m(P(n-4,3,P_5^4,u_1),k)x^{n-2k}\Big).
\end{aligned}
$$

Apparently, since $x>0$, meanwhile, $m(P_{n+2}^l,k)\geq 0$ and $m(P(n-4,3,P_5^4,u_1),k)\geq 0$ hold for all $k\geq 0$, then $H_0(n,x)>0$. Next, we shall verify $C_1(ix)B_2(ix)-C_2(ix)B_1(ix)>0$.

According to the expressions of $C_j(ix)$, $B_j(ix)(j=1,2)$, together with $Z_2(x)f_2+f_1=(Z_2(x))^4$ and $Z_1(x)f_2+f_1=(Z_1(x))^4$, through a series of calculations, we derive

$$
\begin{aligned}
& C_1(ix)B_2(ix)-C_2(ix)B_1(ix)\\
= \;& \Big((Z_2(x))^8(1+(Z_2(x))^2)^2(Z_1(x)g_2+g_1)+(Z_2(x))^{10}(1+(Z_1(x))^2)\\
& (Z_1(x)g_2+g_1)+(Z_1(x))^{2l-10}(1+(Z_2(x))^2)(Z_1(x)g_2+g_1)-(Z_1(x))^8\\
& (1+(Z_1(x))^2)^2(Z_2(x)g_2+g_1)-(Z_1(x))^{10}(1+(Z_2(x))^2)(Z_2(x)g_2+g_1)\\
& -(Z_2(x))^{2l-10}(1+(Z_1(x))^2)(Z_2(x)g_2+g_1)\Big)\Big/(x^2+4)^2.
\end{aligned}
$$

By the help of the computer, we get

$$
\begin{aligned}
Z(x) \;=\;& (Z_2(x))^8(1+(Z_2(x))^2)^2(Z_1(x)g_2+g_1)+(Z_2(x))^{10}(1+(Z_1(x))^2)\\
& (Z_1(x)g_2+g_1)-(Z_1(x))^8(1+(Z_1(x))^2)^2(Z_2(x)g_2+g_1)\\
& -(Z_1(x))^{10}(1+(Z_2(x))^2)(Z_2(x)g_2+g_1)\\
=\;& \sqrt{x^2+4}x^{13}+13\sqrt{x^2+4}x^{11}+63\sqrt{x^2+4}x^9+139\sqrt{x^2+4}x^7\\
& +131\sqrt{x^2+4}x^5+28\sqrt{x^2+4}x^3-10\sqrt{x^2+4}x.
\end{aligned}
$$

Let $H_0(l,x)=(Z_2(x))^{2l-10}(1+(Z_1(x))^2)(Z_2(x)g_2+g_1)-(Z_1(x))^{2l-10}(1+(Z_2(x))^2)(Z_1(x)g_2+g_1)$. It suffices to show $Z(x)>H_0(l,x)$ holds for $x>0$. Take the derivative of $H_0(l,x)$ with respect to l, let $H_0'(l,x)$ denote the derived function. We claim that $H_0(l,x)$ is decreasing on l.

Claim. For $6\leq l\leq \frac{n+1}{2}$ and any given x with $x>0$, the function $H_0(l,x)$ is decreasing on l.

Proof. Clearly, $Z_1(x) > 1$ and $Z_2(x) < 0$. Moreover, since $Z_1(x) \cdot Z_2(x) = -1$, then $\ln(Z_1(x)) + \ln(-Z_2(x)) = \ln(Z_1(x) \cdot (-Z_2(x))) = 0$, which implies that $\ln(-Z_2(x)) = -\ln(Z_1(x))$. Accordingly,

$$\begin{aligned} H_0'(l,x) &= 2(1+(Z_1(x))^2)(Z_2(x)g_2+g_1)(Z_2(x))^{2l-10}\ln(-Z_2(x)) \\ &\quad -2(1+(Z_2(x))^2)(Z_1(x)g_2+g_1)(Z_1(x))^{2l-10}\ln(Z_1(x)) \\ &= -2\ln(Z_1(x))\Big((1+(Z_2(x))^2)(Z_1(x)g_2+g_1)(Z_1(x))^{2l-10} \\ &\quad -(1+(Z_1(x))^2)(-Z_2(x)g_2-g_1)(Z_2(x))^{2l-10}\Big). \end{aligned}$$

Make full use of the computer, we obtain

$$\begin{aligned} & Z_1(x)g_2+g_1 \\ = \ & \frac{1}{2}x^{10} + \frac{1}{2}\sqrt{x^2+4}x^9 + \frac{11}{2}x^8 + \frac{9}{2}\sqrt{x^2+4}x^7 + \frac{41}{2}x^6 + \frac{25}{2}\sqrt{x^2+4}x^5 \\ & + \frac{61}{2}x^4 + \frac{25}{2}\sqrt{x^2+4}x^3 + 16x^2 + 4\sqrt{x^2+4}x + 2 > 0; \\ & (1+(Z_2(x))^2)(Z_1(x)g_2+g_1) - (1+(Z_1(x))^2)(-Z_2(x)g_2-g_1) \\ = \ & x^{10} + 12x^8 + 50x^6 + 84x^4 + 50x^2 + 8 > 0. \end{aligned}$$

Namely, $(1+(Z_2(x))^2)(Z_1(x)g_2+g_1) > 0$ and $(1+(Z_2(x))^2)(Z_1(x)g_2+g_1) > (1+(Z_1(x))^2)(-Z_2(x)g_2-g_1)$. On the other hand, since $Z_1(x) > |Z_2(x)| > 0$, then $(Z_1(x))^{2l-10} > (Z_2(x))^{2l-10} > 0$ for $l \geq 6$. Consequently, we always have $(1+(Z_2(x))^2)(Z_1(x)g_2+g_1)(Z_1(x))^{2l-10} - (1+(Z_1(x))^2)(-Z_2(x)g_2 - g_1)(Z_2(x))^{2l-10} > 0$. Hence $H_0'(l,x) < 0$. That is, $H_0(l,x)$ is decreasing on l.

It follows from the claim that $H_0(l,x) \leq H_0(6,x)$. As $Z(x) - H_0(6,x) = \sqrt{x^2+4}x^{13} + 14\sqrt{x^2+4}x^{11} + 75\sqrt{x^2+4}x^9 + 190\sqrt{x^2+4}x^7 + 224\sqrt{x^2+4}x^5 + 98\sqrt{x^2+4}x^3 + 8\sqrt{x^2+4}x > 0$ for all $x > 0$, we demonstrate that $Z(x) > H_0(6,x) \geq H_0(l,x)$. Therefore, $C_1(ix)B_2(ix) - C_2(ix)B_1(ix) = (Z(x) - H_0(l,x))/(x^2+4)^2 > 0$.

Up to now, we have established that $C_1(ix)B_2(ix) - C_2(ix)B_1(ix) > 0$, which indicates that $K_0(x) < 0$. Hence $\ln(1+\frac{K_0(x)}{H_0(n,x)}) < \ln 1 = 0$. Namely, we have $\ln\frac{C_1(ix)(Y_1(ix))^{n+2}+C_2(ix)(Y_2(ix))^{n+2}}{B_1(ix)(Y_1(ix))^{n+2}+B_2(ix)(Y_2(ix))^{n+2}} < \ln\frac{C_1(ix)(Y_1(ix))^{n}+C_2(ix)(Y_2(ix))^{n}}{B_1(ix)(Y_1(ix))^{n}+B_2(ix)(Y_2(ix))^{n}}$. Thus

$$\ln\frac{C_1(ix)(Y_1(ix))^n + C_2(ix)(Y_2(ix))^n}{B_1(ix)(Y_1(ix))^n + B_2(ix)(Y_2(ix))^n} \leq \ln\frac{C_1(ix)(Y_1(ix))^{11} + C_2(ix)(Y_2(ix))^{11}}{B_1(ix)(Y_1(ix))^{11} + B_2(ix)(Y_2(ix))^{11}}$$

for $n \geq 11$. This yields that for $6 \leq l \leq \frac{n+1}{2}$,

$$\begin{aligned}
& ME(P(n-4,3,P_5^4,u_1)) - ME(P_n^l) \\
= \quad & \frac{2}{\pi}\int_0^\infty \ln \frac{C_1(ix)(Y_1(ix))^n + C_2(ix)(Y_2(ix))^n}{B_1(ix)(Y_1(ix))^n + B_2(ix)(Y_2(ix))^n} dx \\
\leq \quad & \frac{2}{\pi}\int_0^\infty \ln \frac{C_1(ix)(Y_1(ix))^{11} + C_2(ix)(Y_2(ix))^{11}}{B_1(ix)(Y_1(ix))^{11} + B_2(ix)(Y_2(ix))^{11}} dx \\
= \quad & ME(P(7,3,P_5^4,u_1)) - ME(P_{11}^l).
\end{aligned}$$

When $n = 11$, then $l = 6$. By computer-aided calculations, we arrive at $ME(P(7,3,P_5^4,u_1)) = 13.75635$, $ME(P_{11}^6) = 13.77695$. Hence $ME(P(n-4,3,P_5^4,u_1)) - ME(P_n^l) \leq ME(P(7,3,P_5^4,u_1)) - ME(P_{11}^6) < 0$, i.e., $ME(P(n-4,3,P_5^4,u_1)) < ME(P_n^l)$. The proof is thus completed. ∎

Based on the lemmas we established, we can now state our main results.

Theorem 1. *Let $n \geq 9$ be odd and l be even. If G is an arbitrary graph in $\mathcal{B}_{n,n}$ other than the graphs $P_n^l (4 \leq l \leq \frac{n+1}{2})$, then $ME(G) < ME(P_n^l)$.*

Proof. Let G be an arbitrary graph in $\mathcal{B}_{n,n}$ other than the graphs $P_n^l (4 \leq l \leq \frac{n+1}{2})$. Suppose the girth of G is $g = g(G)$.

If $n = 9$, then $l = 4$, by Lemma 4 and Remark 2 after Lemma 9, it's easy to obtain, for such a graph G, that $ME(G) \leq ME(P_9^g) \leq ME(P_9^4)$. Furthermore, the equalities can not hold simultaneously. Hence $ME(G) < ME(P_9^4)$.

If $n = 11$, then $l = 4, 6$. Since $ME(P_{11}^4) > ME(P_{11}^6)$, it suffices to show $ME(G) < ME(P_{11}^6)$. If $g \geq 6$, then according to Lemma 4 and Remark 2 after Lemma 9, there has no need to elaborate. If $g = 4$, then we should only consider the graph $P(7,3,P_5^4,u_1)$ on the basis of the lemmas 11–19. Applying Lemma 21 directly, we get $ME(P(7,3,P_5^4,u_1)) < ME(P_{11}^6)$.

If $n \geq 13$, for $g > \frac{n+1}{2}$, we have $ME(G) \leq ME(P_n^g) < ME(P_n^{\frac{n+1}{2}}) \leq ME(P_n^l)$. For $g = \frac{n+1}{2}$, since $G \ncong P_n^{\frac{n+1}{2}}$, we have $ME(G) < ME(P_n^{\frac{n+1}{2}}) \leq ME(P_n^l)$. For $g < \frac{n+1}{2} \leq n-5$, putting Lemmas 11–19 together with Lemma 21, we can show $ME(G) < ME(P_n^l)$.

The theorem is thus proved. ∎

Combining Theorem 1 with Remark 2 after Lemma 9, it's not difficult to obtain the key point of our paper.

Theorem 2. *Let $n \geq 9$ be odd. Then we have*
(i) If $n \equiv 3$ (mod 4), P_n^4, P_n^6, $\ldots$, $P_n^{\frac{n+1}{2}}$ are the graphs in $\mathcal{B}_{n,n}$ with the first

$\frac{n-3}{4}$ *largest matching energies;*

(ii) If $n \equiv 1 \pmod 4$*,* P_n^4*,* P_n^6*,* $\ldots$*,* $P_n^{\frac{n-1}{2}}$ *are the graphs in* $\mathcal{B}_{n,n}$ *with the first* $\frac{n-5}{4}$ *largest matching energies.*

4. Conclusion

In this paper, we established the graphs in $\mathcal{B}_{n,n}$ with the first $\lfloor \frac{n-3}{4} \rfloor$ largest matching energies. They all have the form of P_n^l for some l. Among these graphs, the graph P_n^6 plays an important role in unicyclic graphs. In [45], the authors determined that P_n^6 is the only graph which attains the maximum value of the energy among all the bipartite unicyclic graphs for $n \geq 16$. Furthermore, it's the graph having maximal energy among all unicyclic graphs (see [4] and [44]). While in this paper, for odd n, we conclude that P_n^6 has the second maximal matching energy in $\mathcal{B}_{n,n}$ when $n \geq 11$.

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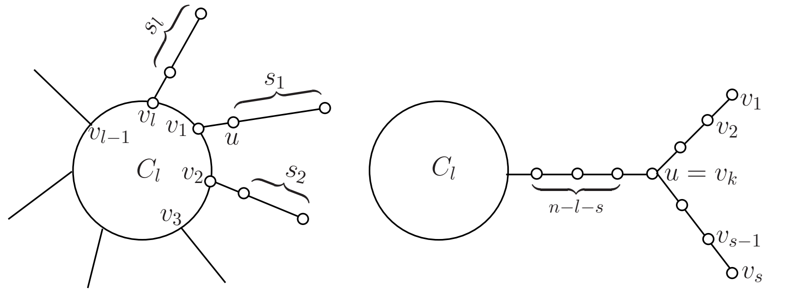
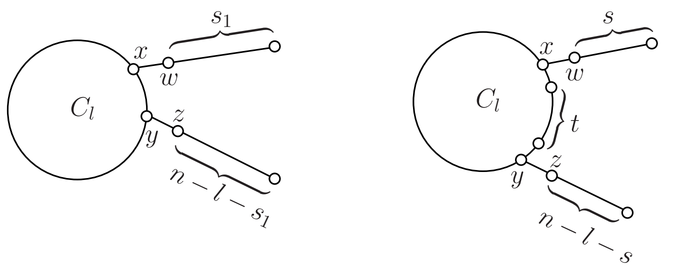


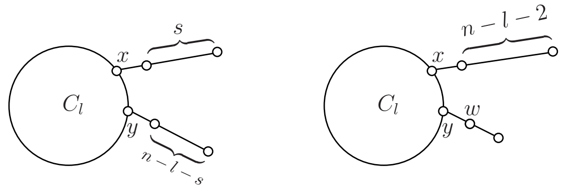
$C_l(P_{s_1+1},\ldots,P_{s_l+1})$ $\quad$ $P(s,k,P^l_{n-s+1},u)$

Fig 1 The graphs $C_l(P_{s_1+1},\ldots,P_{s_l+1})$ and $P(s,k,P^l_{n-s+1},u)$.



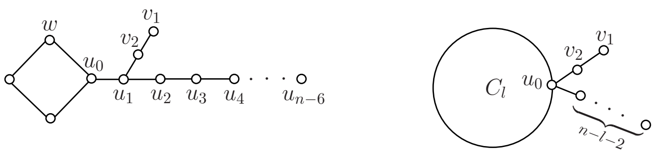
$C_l(P_{s_1+1},P_{n-l-s_1+1},P_1,\ldots,P_1)$ $\quad$ $C_l(P_{s+1},\underbrace{P_1,\ldots,P_1}_{t},P_{n-l-s+1},P_1,\ldots,P_1)$

Fig 2 The graphs $C_l(P_{s_1+1},P_{n-l-s_1+1},P_1,\ldots,P_1)$ and $C_l(P_{s+1},\underbrace{P_1,\ldots,P_1}_{t},P_{n-l-s+1},P_1,\ldots,P_1)$.

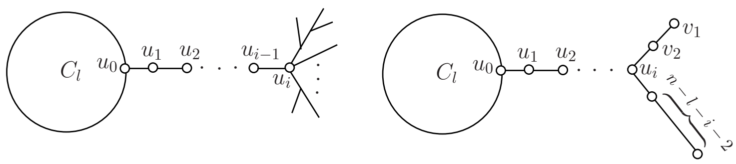


$C_l(P_{s+1}, P_{n-l-s+1}, P_1, \ldots, P_1)$ $C_l(P_{n-l-1}, P_3, P_1, \ldots, P_1)$

Fig 3 The graphs used in Lemma 12.

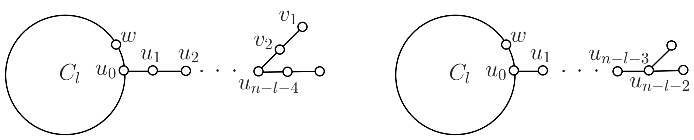


$P(n-4, 3, P_5^4, u_1)$ $P(n-l+1, 3, C_l, u_0)$



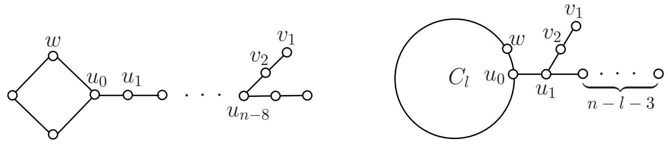
G $P(n-l-i+1, 3, P_{l+i}^l, u_i)$

Fig 4 Some graphs needed in our paper.



$P(5, 3, P_{n-4}^l, u_{n-l-4})$ $P(3, 2, P_{n-2}^l, u_{n-l-2})$

Fig 5 The graphs $P(5, 3, P_{n-4}^l, u_{n-l-4})$ and $P(3, 2, P_{n-2}^l, u_{n-l-2})$.



$P(5, 3, P_{n-4}^4, u_{n-8})$ $P(n-l, 3, P_{l+1}^l, u_1)$

Fig 6 The graphs $P(5, 3, P_{n-4}^4, u_{n-8})$ and $P(n-l, 3, P_{l+1}^l, u_1)$.