Bounds on the Matching Energy of Unicyclic Odd-cycle Graphs

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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. Referring to graphs with no even cycles as odd-cycle graphs, denote by $\mathcal{O}_n$ the class of odd-cycle graphs of order n, and $\mathcal{O}_{n,m}$ the class of graphs in $\mathcal{O}_n$ with m edges. Especially, we call the graphs in $\mathcal{O}_{n,n}$ as unicyclic odd-cycle graphs. In this paper, we determine the graphs with the second through the fourth maximal matching energies in $\mathcal{O}_{n,n}$ when n is odd, and establish the graphs with the maximal matching energy in $\mathcal{O}_{n,n}$ when n is even. It is interesting that the extremal graphs for matching energy are of the form P_n^{ℓ} for some values of ℓ, which are related to the extremal graph (i.e., P_n^6) having the maximal energy among unicyclic graphs.

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 [16,39] include the (general) Randić index [34,35], the (general) zeroth–

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order Randić index [22, 23], the Zagreb indices [20, 41], the ABC index [19], and so on. Distance–based indices [44] include the Balaban index [7], the Wiener index [11] the Wiener polarity index [38], the Harary index [42] and so on. Eigenvalues of graphs [45, 46], various of graph energies [3, 8, 9], the HOMO–LUMO index [33] belong to spectrum–based indices. Actually, there are also some topological indices defined on both degrees and distances, such as degree distance [13] and graph entropies [4, 10, 29].

In 1977, Gutman [14] 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 theory of graph energy is well developed. The graph energy has been rather widely studied by theoretical chemists and mathematicians. For details, we refer the book on graph energy [36] and some recent references [24, 25, 37].

Throughout this paper, all graphs under our consideration are finite, connected, and simple. We first introduce some elementary notations and terminology that will be used in the sequel. With regard to other notations, the readers are referred to the book [2].

By convention, denote by P_n, C_n, and S_n the path, cycle, and star of order n. $\mathcal{T}_n$ denotes the set of trees with n vertices. The graph obtained by connecting a vertex of C_ℓ with a leaf of $P_{n-\ell}$ is denoted by P_n^ℓ. We refer to graphs with no even cycles as *odd-cycle graphs*. Let $\mathcal{O}_n$ be the class of odd-cycle graphs of order n, and $\mathcal{O}_{n,m}$ be the class of graphs in $\mathcal{O}_n$ with m edges. Especially, we call the graphs in $\mathcal{O}_{n,n}$ as *unicyclic odd-cycle graphs*. It is easy to get the following property of odd-cycle graphs [31].

Proposition 1.1. *For any graph $G \in \mathcal{O}_{n,m}$, since there are no even cycles in it, any two cycles in G have at most one common vertex. So we have $n - 1 \leq m \leq \frac{3}{2}(n-1)$.*

Let G be a graph with n vertices and m edges. A *matching* in 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

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

In [21], 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 1.2 ([21])**.** *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*

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

Obviously, by the monotonicity of the logarithm function, formula (1) implies that the matching energy of a graph G is a monotonically increasing function of any $m(G,k)$. In particular, 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 define a *quasi-order* $\succeq$ as follows: If G_1 and G_2 are two graphs, then

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

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*, denoted 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, and write $G_1 \succ G_2$. If neither $G_1 \succeq G_2$ nor $G_2 \succeq G_1$, then 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 Eqs.(1) and (2), $G_1 \succeq G_2 \Longrightarrow ME(G_1) \geq ME(G_2)$ and $G_1 \succ G_2 \Longrightarrow ME(G_1) > ME(G_2)$.

In [21], 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. On the chemical applications of matching energy, for more details see [17].

As the research of extremal energy is an amusing work, the study on extremal matching energy is also interesting. In [21], 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 [28], Ji et al. characterized the graphs with the extremal matching energy among all bicyclic graphs, while Chen and Shi [6] proved the same extremal results for tricyclic graphs. In [5], Chen et al. characterized the graphs with minimal matching energy among all unicyclic and bicyclic graphs with a given diameter d. For some more extremal results on matching energy of graphs see [32, 43].

In [31], the authors studied the extremal skew energy of digraphs with no even cycles. Motivated by this, we investigate the extremal values of matching energy of unicyclic odd-cycle graphs. In this paper, we determine the graphs with the second through the fourth maximal matching energies in $\mathcal{O}_{n,n}$ when n is odd, and give the graphs with the maximal matching energy in $\mathcal{O}_{n,n}$ when n is even.

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 the maximal energy of unicyclic graphs (see [1] and [26]).

2 Preliminary

In this section, we list some previously known results that will be needed in the next two sections.

Lemma 2.1 ([12, 15]). *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:*

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

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

According to Eq. (4), we get $m(P_1 \cup G, k) = m(G, k)$ directly, where G is an arbitrary graph and P_1 is an isolated vertex.

Lemma 2.2 ([5]). *Let G be a simple graph and H be a subgraph (resp. proper subgraph) of G. Then $G \succeq H$ (resp. $\succ H$).*

Lemma 2.3 ([30]). *Let n, ℓ be positive integers, $n > \ell \geq 3$. Denote by $\mathcal{U}_{\ell,n}$ the set of unicyclic graphs with n vertices and a cycle of length ℓ. Then for any graph $G \in \mathcal{U}_{\ell,n}$,*

$$ME(P_n^\ell) \geq ME(G)$$

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

In fact, the authors in [30] proved that $P_n^\ell \succ G$ for any $G \in \mathcal{U}_{\ell,n} \setminus \{P_n^\ell\}$.

Lemma 2.4 ([14,28]). *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 2.5 ([18]). *Let H_1 and H_2 be 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 2.6 ([21]). *If the graph F is a forest, then its matching energy coincides with its energy.*

Lemma 2.7 ([14, 21]). *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 $F \cong P_n$.*

3 Odd n

As we know, $\mathcal{O}_{n,n}$ is the class of connected graphs with n vertices and n edges that contain an odd cycle, say C_ℓ, as a subgraph, where $3 \leq \ell \leq n$. It is known [21] that among all unicyclic graphs on n vertices, C_n has the maximal matching energy. When n is odd, $C_n \in \mathcal{O}_{n,n}$, hence the graph having maximal matching energy in $\mathcal{O}_{n,n}$ is exactly C_n. In this section, we determine the graphs with the second through the fourth maximal matching energies in $\mathcal{O}_{n,n}$ for n being odd. We begin this section with the following lemma.

Lemma 3.1. *Let $n \geq 5$ be odd and t be an even integer, where $0 \leq t \leq n-5$. Then $P_n^{n-t} \succ P_n^{n-t-2}$.*

Proof. When $k = 0$, then clearly, $m(P_n^{n-t}, 0) = m(P_n^{n-t-2}, 0) = 1$. When $1 \leq k \leq \frac{n-1}{2}$, then by Eq. (3), we have

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

and

$$m(P_n^{n-t-2}, k) = m(P_n, k) + m(P_{t+2} \cup P_{n-t-4}, k-1)\,.$$

Since n is odd, while t is even, then both t and $t+2$ are even, both $n-t-2$ and $n-t-4$ are odd. Thus by Lemma 2.4, $P_t \cup P_{n-t-2} \succ P_{t+2} \cup P_{n-t-4}$, which implies that $m(P_t \cup P_{n-t-2}, k-1) \geq m(P_{t+2} \cup P_{n-t-4}, k-1)$. Meanwhile, there exists at least one k_0 such that $m(P_t \cup P_{n-t-2}, k_0) > m(P_{t+2} \cup P_{n-t-4}, k_0)$. Hence $m(P_n^{n-t}, k) \geq m(P_n^{n-t-2}, k)$ for all k, especially, $m(P_n^{n-t}, k_0+1) > m(P_n^{n-t-2}, k_0+1)$. Accordingly, $P_n^{n-t} \succ P_n^{n-t-2}$. □

Remark 1. By Lemma 3.1, we easily see that

$$C_n \succ P_n^{n-2} \succ P_n^{n-4} \succ P_n^{n-6} \succ \ldots \succ P_n^5 \succ P_n^3\,.$$

In fact, when n is odd, then P_n^{n-2}, P_n^{n-4} and P_n^{n-6} are precisely the second, the third, and the fourth maximal graphs in $\mathcal{O}_{n,n}$ with respect to matching energy. We state the following two theorems to prove this fact.

Theorem 3.2. *Let $n \geq 7$ be odd. Then P_n^{n-2} and P_n^{n-4} are the graphs with the second maximal matching energy and the third maximal matching energy in $\mathcal{O}_{n,n}$, respectively.*

Proof. For any graph $G \in \mathcal{O}_{n,n}$ with $G \ncong C_n$, suppose the girth of G is $g(G) = \ell$, where $n \geq 7$ is odd and $3 \leq \ell \leq n-2$.

Case 1. If $G \ncong P_n^{n-2}$, then by Lemma 2.3 and Remark 1, $G \preceq P_n^{\ell} \preceq P_n^{n-2}$. With $G \sim P_n^{\ell}$ and $P_n^{\ell} \sim P_n^{n-2}$ if and only if $G \cong P_n^{n-2}$, a contradiction. Thus $G \prec P_n^{n-2}$. In addition, we have known that $C_n \succ P_n^{n-2}$. Therefore, P_n^{n-2} has the second maximal matching energy in $\mathcal{O}_{n,n}$.

Case 2. If $G \ncong P_n^{n-2}$ and $G \ncong P_n^{n-4}$, then similarly, for $3 \leq \ell \leq n-4$, we have $G \preceq P_n^{\ell} \preceq P_n^{n-4}$. With $G \sim P_n^{\ell}$ and $P_n^{\ell} \sim P_n^{n-4}$ if and only if $G \cong P_n^{n-4}$, a contradiction. Hence $G \prec P_n^{n-4}$.

For $\ell = n-2$, since $G \ncong P_n^{n-2}$, then obviously $G \cong H_1$ or H_2 in Fig. 3.1.
By direct checking, it's easy to verify that $H_1 \prec P_n^{n-4}$ as well as $H_2 \prec P_n^{n-4}$. Therefore, we can always show that $G \prec P_n^{n-4}$. Namely, P_n^{n-4} has the third maximal matching energy in $\mathcal{O}_{n,n}$ since we also have $C_n \succ P_n^{n-2} \succ P_n^{n-4}$.

Combining Case 1 with Case 2, we complete the proof. □

Now we give a supplementary notation and a lemma associated with it, which are needed in our proof.

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. Hence if G has n vertices, then $G(e/j)$ has $n+j$ vertices; if $j=0$, then $G(e/j) = G$; if $j > 0$, then the vertices v_r and v_s are not adjacent in $G(e/j)$. There is a following result on the number of k-matchings of the graph $G(e/j)$.

Lemma 3.3 ([18]). *For all $j \geq 0$,*

$$m(G(e/j+2), k) = m(G(e/j+1), k) + m(G(e/j), k-1)\,.$$

Theorem 3.4. *Let $n \geq 9$ be odd. Then P_n^{n-6} is the graph with the fourth maximal matching energy in $\mathcal{O}_{n,n}$ for $n \geq 11$, and $H_{6,0}$ is the graph with the fourth maximal matching energy in $\mathcal{O}_{9,9}$, where $H_{6,0}$ is shown in Fig. 3.1.*

Proof. For any graph $G \in \mathcal{O}_{n,n}$ with $G \ncong C_n$, let the girth of G be $g(G) = \ell$, where $n \geq 9$ is odd and $3 \leq \ell \leq n-2$. Suppose that $G \ncong P_n^{n-2}$, $G \ncong P_n^{n-4}$, and $G \ncong P_n^{n-6}$.

If $3 \leq \ell \leq n-6$, then similar to Case 1 in Theorem 3.2, we get $G \prec P_n^{n-6}$.

If $\ell = n-2$, i.e., $G \cong H_1$ or H_2, then by simple calculation, we also get $H_1 \prec P_n^{n-6}$ and $H_2 \prec P_n^{n-6}$.

If $\ell = n-4$, then $G \cong H_i$ $(i = 3, 4, \ldots, 20)$ in Fig. 3.1.

Case 1. When $G \cong H_3$ and $n = 9$, then

$$\begin{aligned} m(H_3, k) &= m(T_1, k) + m(P_3 \cup P_3, k-1) + m(P_3, k-2) \\ m(P_n^{n-6}, k) &= m(P_9, k) + m(P_3 \cup P_3, k-1) + m(P_2 \cup P_2, k-2) \end{aligned}$$

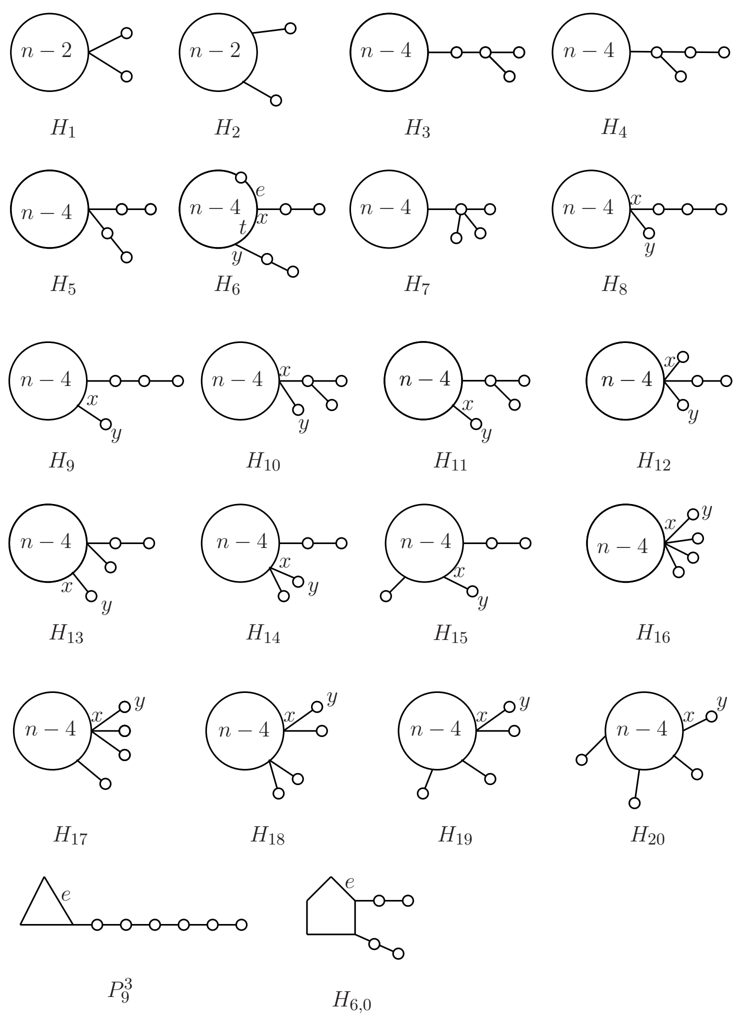

Figure 3.1: The graphs needed in the proof of Theorem 3.2 and Theorem 3.4.

where $T_1 \in \mathcal{T}_9$. Hence $m(H_3, k) \leq m(P_n^{n-6}, k)$ since $m(T_1, k) \leq m(P_9, k)$ and $m(P_3, k-2) \leq m(P_2 \cup P_2, k-2)$. Moreover, $m(H_3, 4) < m(P_n^{n-6}, 4)$ since $m(P_3, 2) < m(P_2 \cup P_2, 2)$. Therefore, $H_3 \prec P_n^{n-6}$ for $n = 9$.

Case 2. When $G \cong H_3$ and $n \geq 11$, then

$$\begin{aligned} m(H_3, k) &= m(T_2, k) + m(P_{n-6} \cup P_3, k-1) + m(P_{n-6}, k-2) \\ m(P_n^{n-6}, k) &= m(P_n, k) + m(P_{n-8} \cup P_5, k-1) + m(P_{n-8} \cup P_4, k-2) \end{aligned}$$

where $T_2 \in \mathcal{T}_n$. Since $n \geq 11$, then $m(T_2, k) \leq m(P_n, k)$, $m(P_{n-6} \cup P_3, k-1) \leq m(P_{n-8} \cup P_5, k-1)$, $m(P_{n-6}, k-2) \leq m(P_{n-8} \cup P_4, k-2)$. Which imply that $m(H_3, k) \leq m(P_n^{n-6}, k)$. Furthermore, since $T_2 \ncong P_n$, there exists some k_0 such that

$m(T_2, k_0) < m(P_n, k_0)$. Thus $m(H_3, k_0) < m(P_n^{n-6}, k_0)$. It follows that $H_3 \prec P_n^{n-6}$ for $n \geq 11$.

Case 3. If $G \cong H_7$, similarly, then we can show that $G \prec P_n^{n-6}$ for $n \geq 9$.

Case 4. If $G \cong H_i\,(i = 8, 9, \ldots, 20)$, then one can check that there always exists some pendent edge of G, say xy, such that x is in the unique cycle of G (see in the figure). Take an edge xz of the unique cycle, such that $G - xz = T_3 (\in \mathcal{T}_n) \prec P_n$ and $G - x - z \preceq P_{n-3}$. Then

$$\begin{aligned} m(G,k) &= m(G - xz, k) + m(G - x - z, k-1) \\ &\leq m(P_n, k) + m(P_{n-3}, k-1) \\ &\leq m(P_n, k) + m(P_{n-8} \cup P_6, k-1) \\ &= m(P_n^{n-6}, k). \end{aligned}$$

In addition, since $G - xz \prec P_n$, there exists some k_0 such that $m(G - xz, k_0) < m(P_n, k_0)$. That is, $m(G, k_0) < m(P_n^{n-6}, k_0)$. Hence $G \prec P_n^{n-6}$.

Case 5. We now only need consider the cases for $G \cong H_4$, H_5 or H_6. For the graph H_6, let the two 3-degree vertices be x and y, respectively. Suppose that the number of vertices in the unique cycle between x and y is t, where $0 \leq t \leq \lfloor \frac{n-6}{2} \rfloor$. Then it's obviously that H_6 arrives at the maximal matching energy if and only if $t = 0$ (i.e., H_6 has larger matching energy when $t = 0$ than that when $1 \leq t \leq \lfloor \frac{n-6}{2} \rfloor$). Hence in the sequel, whenever we mention the graph H_6, it implies that $t = 0$. Accordingly, it's easy to check that $H_6 \succ H_5$. Simultaneously, since

$$m(H_6, k) = m(P_{n-2}^{n-4} \cup P_2, k) + m(P_{n-4}, k-1) + m(P_{n-5}, k-2)$$

whereas

$$m(H_4, k) = m(P_{n-2}^{n-4} \cup P_2, k) + m(P_{n-4}, k-1) + m(P_{n-6}, k-2)$$

then $H_6 \succ H_4$ as $P_{n-5} \succ P_{n-6}$. Consequently, it suffices to compare P_n^{n-6} with H_6.

By the definition of $G(e/j)$, $P_n^{n-6} = P_9^3(e/n-9)$ and $H_6 = H_{6,0}(e/n-9)$, where P_9^3 and $H_{6,0}$ are depicted in Fig. 3.1. In [6], we have shown that $\alpha(G(e/j+2), x) = x\alpha(G(e/j+1), x) - \alpha(G(e/j), x)$. That is, both $\alpha(P_n^{n-6}, x)$ and $\alpha(H_6, x)$ 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 $Y_1(x)Y_2(x) = 1$. We obtain the values of $C_i(x)$ $(i = 1, 2)$ as follows.

By simple calculations, we get:

$m(P_9^3, 0) = 1$, $m(P_9^3, 1) = 9$, $m(P_9^3, 2) = 26$, $m(P_9^3, 3) = 26$, $m(P_9^3, 4) = 6$, $m(P_9^3, k) = 0$ for $k \geq 5$;

$m(P_{10}^4, 0) = 1$, $m(P_{10}^4, 1) = 10$, $m(P_{10}^4, 2) = 34$, $m(P_{10}^4, 3) = 46$, $m(P_{10}^4, 4) = 22$, $m(P_{10}^4, 5) = 2$, $m(P_{10}^4, k) = 0$ for $k \geq 6$;

$m(H_{6,0}, 0) = 1$, $m(H_{6,0}, 1) = 9$, $m(H_{6,0}, 2) = 25$, $m(H_{6,0}, 3) = 25$, $m(H_{6,0}, 4) = 7$, $m(H_{6,0}, k) = 0$ for $k \geq 5$;

$m(H_{6,0}(e/1), 0) = 1$, $m(H_{6,0}(e/1), 1) = 10$, $m(H_{6,0}(e/1), 2) = 33$, $m(H_{6,0}(e/1), 3) = 43$, $m(H_{6,0}(e/1), 4) = 20$, $m(H_{6,0}(e/1), 5) = 2$, $m(H_{6,0}(e/1), k) = 0$ for $k \geq 6$.

Thus, the initial values are:

$$\begin{aligned}
\alpha(P_9^3, x) &= x^9 - 9x^7 + 26x^5 - 26x^3 + 6x \\
&= C_1(x)(Y_1(x))^9 + C_2(x)(Y_2(x))^9 \\
\alpha(P_{10}^4, x) &= x^{10} - 10x^8 + 34x^6 - 46x^4 + 22x^2 - 2 \\
&= C_1(x)(Y_1(x))^{10} + C_2(x)(Y_2(x))^{10} \\
\alpha(H_{6,0}, x) &= x^9 - 9x^7 + 25x^5 - 25x^3 + 7x \\
&= C_1'(x)(Y_1(x))^9 + C_2'(x)(Y_2(x))^9 \\
\alpha(H_{6,0}(e/1), x) &= x^{10} - 10x^8 + 33x^6 - 43x^4 + 20x^2 - 2 \\
&= C_1'(x)(Y_1(x))^{10} + C_2'(x)(Y_2(x))^{10}.
\end{aligned}$$

By solving the above equalities, we get

$$\begin{aligned}
C_1(x) &= \frac{Y_1(x)\alpha(P_{10}^4, x) - \alpha(P_9^3, x)}{(Y_1(x))^{11} - (Y_1(x))^9} \\
C_2(x) &= \frac{Y_2(x)\alpha(P_{10}^4, x) - \alpha(P_9^3, x)}{(Y_2(x))^{11} - (Y_2(x))^9} \\
C_1'(x) &= \frac{Y_1(x)\alpha(H_{6,0}(e/1), x) - \alpha(H_{6,0}, x)}{(Y_1(x))^{11} - (Y_1(x))^9}
\end{aligned}$$

$$C'_2(x) = \frac{Y_2(x)\alpha(H_{6,0}(e/1),x) - \alpha(H_{6,0},x)}{(Y_2(x))^{11} - (Y_2(x))^9}.$$

Namely, $\alpha(P_n^{n-6},x) = C_1(x)(Y_1(x))^n + C_2(x)(Y_2(x))^n$ and $\alpha(H_6,x) = C'_1(x)(Y_1(x))^n + C'_2(x)(Y_2(x))^n$.

Similar to the calculation in [6], we have

$$\begin{aligned} ME(P_n^{n-6}) - ME(H_6) &= \frac{2}{\pi}\int_0^\infty \ln\frac{\alpha(P_n^{n-6},ix)}{\alpha(H_6,ix)}dx \\ &= \frac{2}{\pi}\int_0^\infty \ln\frac{C_1(ix)(Y_1(ix))^n + C_2(ix)(Y_2(ix))^n}{C'_1(ix)(Y_1(ix))^n + C'_2(ix)(Y_2(ix))^n}\,dx \end{aligned}$$

where $i^2=-1$, $Y_1(ix) = \frac{x+\sqrt{x^2+4}}{2}i$ and $Y_2(ix) = \frac{x-\sqrt{x^2+4}}{2}i$.

We now define $Z_1(x) = -iY_1(x) = \frac{x+\sqrt{x^2+4}}{2}$ and $Z_2(x) = -iY_2(x) = \frac{x-\sqrt{x^2+4}}{2}$, i.e., $Y_1(ix) = iZ_1(x)$ and $Y_2(ix) = iZ_2(x)$. In addition, we set

$$\begin{aligned} f_1 &= i\alpha(P_9^3,ix) = -x^9 - 9x^7 - 26x^5 - 26x^3 - 6x \\ f_2 &= \alpha(P_{10}^4,ix) = -x^{10} - 10x^8 - 34x^6 - 46x^4 - 22x^2 - 2 \\ g_1 &= i\alpha(H_{6,0},ix) = -x^9 - 9x^7 - 25x^5 - 25x^3 - 7x \\ g_2 &= \alpha(H_{6,0}(e/1),ix) = -x^{10} - 10x^8 - 33x^6 - 43x^4 - 20x^2 - 2\,. \end{aligned}$$

It follows that

$$\begin{aligned} C_1(ix) &= \frac{Z_1(x)f_2 + f_1}{-(Z_1(x))^9((Z_1(x))^2+1)} \\ C_2(ix) &= \frac{Z_2(x)f_2 + f_1}{-(Z_2(x))^9((Z_2(x))^2+1)} \\ C'_1(ix) &= \frac{Z_1(x)g_2 + g_1}{-(Z_1(x))^9((Z_1(x))^2+1)} \\ C'_2(ix) &= \frac{Z_2(x)g_2 + g_1}{-(Z_2(x))^9((Z_2(x))^2+1)}\,. \end{aligned}$$

When n is odd, since $Y_1(ix)\cdot Y_2(ix) = 1$, $Z_1(x)\cdot Z_2(x) = -1$, $Z_1(x)+Z_2(x) = x$, and $Z_1(x) - Z_2(x) = \sqrt{x^2+4}$,

$$\ln\frac{C_1(ix)(Y_1(ix))^{n+2} + C_2(ix)(Y_2(ix))^{n+2}}{C'_1(ix)(Y_1(ix))^{n+2} + C'_2(ix)(Y_2(ix))^{n+2}} - \ln\frac{C_1(ix)(Y_1(ix))^n + C_2(ix)(Y_2(ix))^n}{C'_1(ix)(Y_1(ix))^n + C'_2(ix)(Y_2(ix))^n}$$

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

where

$$
\begin{aligned}
K_0(x) &= \Big(C_1(ix)C_2'(ix) - C_2(ix)C_1'(ix)\Big)\Big((Y_1(ix))^2 - (Y_2(ix))^2\Big) \\
&= (f_2g_1 - f_1g_2)x \\
&= x^{14} + 12x^{12} + 52x^{10} + 102x^8 + 92x^6 + 32x^4 + 2x^2
\end{aligned}
$$

and

$$
\begin{aligned}
H_0(n,x) &= \Big(C_1(ix)(Y_1(ix))^n + C_2(ix)(Y_2(ix))^n\Big)\cdot \\
&\quad \Big(C_1'(ix)(Y_1(ix))^{n+2} + C_2'(ix)(Y_2(ix))^{n+2}\Big) \\
&= \alpha(P_n^{n-6}, ix)\cdot \alpha(H_6(e/2), ix) \\
&= \left(\sum_{k\geq 0}(-1)^k m(P_n^{n-6}, k)(ix)^{n-2k}\right)\cdot \\
&\quad \left(\sum_{k\geq 0}(-1)^k m(H_6(e/2), k)(ix)^{(n+2)-2k}\right) \\
&= \left(i^n\sum_{k\geq 0} m(P_n^{n-6}, k)x^{n-2k}\right)\left(i^{n+2}\sum_{k\geq 0} m(H_6(e/2), k)x^{(n+2)-2k}\right) \\
&= \left(\sum_{k\geq 0} m(P_n^{n-6}, k)x^{n-2k}\right)\left(\sum_{k\geq 0} m(H_6(e/2), k)x^{(n+2)-2k}\right).
\end{aligned}
$$

Obviously, $K_0(x) > 0$. Moreover, $H_0(n,x) > 0$ since $x > 0$, $m(P_n^{n-6}, k) \geq 0$ and $m(H_6(e/2), k) \geq 0$ for all k. Hence $\frac{K_0(x)}{H_0(n,x)} > 0$, which deduces that $\ln\Big(1 + \frac{K_0(x)}{H_0(n,x)}\Big) > \ln 1 = 0$. That is,

$$
\ln\frac{C_1(ix)(Y_1(ix))^{n+2} + C_2(ix)(Y_2(ix))^{n+2}}{C_1'(ix)(Y_1(ix))^{n+2} + C_2'(ix)(Y_2(ix))^{n+2}} > \ln\frac{C_1(ix)(Y_1(ix))^{n} + C_2(ix)(Y_2(ix))^{n}}{C_1'(ix)(Y_1(ix))^{n} + C_2'(ix)(Y_2(ix))^{n}}.
$$

Thus, when $n \geq 11$,

$$
\int_0^\infty \ln\frac{\alpha(P_n^{n-6}, ix)}{\alpha(H_6, ix)}dx \geq \int_0^\infty \ln\frac{\alpha(P_{11}^5, ix)}{\alpha(H_{6,0}(e/2), ix)}dx\,.
$$

By computer-aided calculations, we get $ME(P_{11}^5) = 13.74411$ and $ME(H_{6,0}(e/2)) = 13.72523$. Then

$$
\int_0^\infty \ln\frac{\alpha(P_{11}^5, ix)}{\alpha(H_{6,0}(e/2), ix)}dx = \frac{\pi}{2}\big[ME(P_{11}^5) - ME(H_{6,0}(e/2))\big] > 0\,.
$$

It follows that $\int_0^\infty \ln\frac{\alpha(P_n^{n-6}, ix)}{\alpha(H_6, ix)}dx > 0$. Namely,

$$
ME(P_n^{n-6}) - ME(H_6) = \frac{2}{\pi}\int_0^\infty \ln\frac{\alpha(P_n^{n-6}, ix)}{\alpha(H_6, ix)}dx > 0\,.
$$

Therefore, $ME(P_n^{n-6}) > ME(H_6)$ holds for odd n with $n \geq 11$. Consequently, combining with Remark 1, we prove that the graph P_n^{n-6} has the fourth maximal matching energy in $\mathcal{O}_{n,n}$ for odd n with $n \geq 11$.

On the other hand, when $n = 9$, by computer-aided calculations, we get $ME(P_9^3)$ $= 11.12709$, $ME(H_{6,0}) = 11.14211$. Then $ME(P_9^3) < ME(H_{6,0})$. Hence, according to Cases 1-5 and Theorem 3.2, when $n = 9$, the graph $H_{6,0}$ has the fourth maximal matching energy in $\mathcal{O}_{9,9}$.

By this, the proof of Theorem 3.4 has been completed. □

4 Even n

The aim of this section is to discuss the case of even n. The section starts with a result analogous to Lemma 3.1, followed by characterizing the graphs with maximal matching energy in $\mathcal{O}_{n,n}$ when n is even. Moreover, a good property about the ordering in Remark 2 is also obtained.

Lemma 4.1. *Let $n \geq 6$ be even and t be an odd integer with $1 \leq t \leq n-5$. Then $P_n^{n-t} \prec P_n^{n-t-2}$ for $1 \leq t < \frac{n-4}{2}$; $P_n^{n-t} \sim P_n^{n-t-2}$ for $t = \frac{n-4}{2}$; $P_n^{n-t} \succ P_n^{n-t-2}$ for $\frac{n-4}{2} < t \leq n-5$.*

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

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

and

$$m(P_n^{n-t-2}, k) = m(P_n, k) + m(P_{t+2} \cup P_{n-t-4}, k-1)\,.$$

Since n is even but t is odd, then t, $t+2$, $n-t-2$, $n-t-4$ are all odd. If $t \leq n-t-2$ and $t+2 \leq n-t-4$, namely, $t \leq \frac{n-6}{2}$, then by Lemma 2.4, $P_t \cup P_{n-t-2} \prec P_{t+2} \cup P_{n-t-4}$. If $t \leq n-t-2$, $t+2 > n-t-4$ and $t \leq n-t-4$, namely, $\frac{n-6}{2} < t \leq \frac{n-4}{2}$, then $P_t \cup P_{n-t-2} \preceq P_{t+2} \cup P_{n-t-4}$. If $t \leq n-t-2$, $t+2 > n-t-4$ and $t > n-t-4$, namely, $\frac{n-4}{2} < t \leq \frac{n-2}{2}$, then $P_t \cup P_{n-t-2} \succ P_{t+2} \cup P_{n-t-4}$. If $t > n-t-2$ and $t+2 > n-t-4$, namely, $t > \frac{n-2}{2}$, then $P_t \cup P_{n-t-2} \succ P_{t+2} \cup P_{n-t-4}$. In summary, if $1 \leq t < \frac{n-4}{2}$, then $P_t \cup P_{n-t-2} \prec P_{t+2} \cup P_{n-t-4}$. If $t = \frac{n-4}{2}$, then $P_t \cup P_{n-t-2} = P_{t+2} \cup P_{n-t-4}$. If

$\frac{n-4}{2} < t \leq n-5$, then $P_t \cup P_{n-t-2} \succ P_{t+2} \cup P_{n-t-4}$. This yields $P_n^{n-t} \prec P_n^{n-t-2}$ when $1 \leq t < \frac{n-4}{2}$, $P_n^{n-t} \sim P_n^{n-t-2}$ when $t = \frac{n-4}{2}$, and $P_n^{n-t} \succ P_n^{n-t-2}$ when $\frac{n-4}{2} < t \leq n-5$. This completes the proof. □

Remark 2. According to Lemma 4.1, we know that
$P_n^{n-1} \prec P_n^{n-3} \prec P_n^{n-5} \prec \cdots \prec P_n^{\frac{n}{2}+5} \prec P_n^{\frac{n}{2}+3} \prec P_n^{\frac{n}{2}+1} \succ P_n^{\frac{n}{2}-1} \succ P_n^{\frac{n}{2}-3} \succ \cdots \succ P_n^7 \succ P_n^5 \succ P_n^3$ for $n \equiv 0 \pmod 4$,
and
$P_n^{n-1} \prec P_n^{n-3} \prec P_n^{n-5} \prec \cdots \prec P_n^{\frac{n}{2}+6} \prec P_n^{\frac{n}{2}+4} \prec P_n^{\frac{n}{2}+2} \sim P_n^{\frac{n}{2}} \succ P_n^{\frac{n}{2}-2} \succ P_n^{\frac{n}{2}-4} \succ \cdots \succ P_n^7 \succ P_n^5 \succ P_n^3$ for $n \equiv 2 \pmod 4$.

Bearing in mind Lemma 2.3, and making full use of the above remark, the next theorem follows immediately.

Theorem 4.2. *If $n \equiv 0 \pmod 4$, then the graph with maximal matching energy in $\mathcal{O}_{n,n}$ is $P_n^{\frac{n}{2}+1}$. If $n \equiv 2 \pmod 4$, then the graphs with maximal matching energy in $\mathcal{O}_{n,n}$ are $P_n^{\frac{n}{2}}$ and $P_n^{\frac{n}{2}+2}$.*

In addition, in connection with the ordering in Remark 2, we find that $P_n^t \sim P_n^{n-t+2}$.

Proposition 4.3. *Let n be even and t be odd with $3 \leq t \leq n-1$. Then $P_n^t \sim P_n^{n-t+2}$.*

Proof. For all $k \geq 0$, on the basis of Eq. (3), one obtains that

$$\begin{aligned} m(P_n^t, k) &= m(P_n, k) + m(P_{t-2} \cup P_{n-t}, k-1) \\ m(P_n^{n-t+2}, k) &= m(P_n, k) + m(P_{t-2} \cup P_{n-t}, k-1)\,. \end{aligned}$$

Apparently, $m(P_n^t, k) = m(P_n^{n-t+2}, k)$ holds for all k, which implies $P_n^t \sim P_n^{n-t+2}$. □

Similar to the case of n being odd, when n is even, with respect to matching energy, we can apply the same method to consider the second maximal graph, the third maximal graph, and so on.

5 Summary

In this paper, when n is odd, only the first four maximal graphs with regard to matching energy have been taken into account. Actually, we conjecture that the graphs P_n^ℓ are the second through the $(\lfloor \frac{n}{2} \rfloor /2+1)$-th maximal graphs when the odd integer ℓ ranges from $n-2$ to $\lceil \frac{n}{2} \rceil$. Verifying this claim will be one of our tasks in the future.

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