The Maximal Matching Energy of Tricyclic Graphs

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Abstract

Gutman and Wagner proposed the concept of the matching energy (ME) and pointed out that the chemical applications of ME go back to the 1970s. Let G be a simple graph of 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 μ_i $(i = 1, 2, \ldots, n)$. Gutman and Cvetkoić determined the tricyclic graphs on n vertices with maximal number of matchings by a computer search for small values of n and by an induction argument for the rest. Based on this result, in this paper, we characterize the graphs with the maximal value of matching energy among all tricyclic graphs, and completely determine the tricyclic graphs with the maximal matching energy. We prove our result by using Coulson-type integral formula of matching energy, which is similar as the method to comparing the energies of two quasi-order incomparable graphs.

1 Introduction

In this paper, all graphs under our consideration are finite, connected, undirected and simple. For more notations and terminologies that will be used in the sequel, we refer to [2]. Let G be such a graph, and let n and m be the number of its vertices and

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edges, respectively. 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. Denote by $m(G,k)$ 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 $m(G,0)=1$. The matching polynomial of graph G is defined as

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

In 1977, Gutman [4] proposed the concept of graph energy. The energy of 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 [24] and reviews [8, 10]. Recently, Gutman and Wagner [13] defined the matching energy of a graph G based on the zeros of its matching polynomial [3, 5].

Definition 1.1 *Let G be a simple graph with order n, and $\mu_1,\mu_2,\ldots,\mu_n$ be the zeros of its matching polynomial. Then,*

$$ME(G)=\sum_{i=1}^{n}|\mu_i|. \tag{1.1}$$

Moreover, Gutman and Wagner [13] 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 [1, 11, 12].

An important tool of graph energy is the Coulson-type integral formula [4] (with regard to G be a tree T):

$$E(T)=\frac{2}{\pi}\int_0^{\infty}\frac{1}{x^2}\ln\Big[\sum_{k\geq 0}m(T,k)x^{2k}\Big]dx, \tag{1.2}$$

which is valid for any tree T (or, more generally, for any forest). Being similar to Eq.(1.2), the matching energy also has a beautiful formula as follows [13].

Proposition 1.2 *Let G be a simple graph of order n, and $m(G,k)$ be the number of its k-matchings, $k = 0, 1, 2, \ldots, \lfloor \frac{n}{2} \rfloor$. The matching energy of G is given by*

$$ME = ME(G) = \frac{2}{\pi} \int_0^\infty \frac{1}{x^2} \ln \Big[\sum_{k \geq 0} m(G,k) x^{2k} \Big] dx. \tag{1.3}$$

Combining Eq.(1.2) with Eq.(1.3), it immediately follows that: if G is a forest, then its matching energy coincides with its energy.

Formula (1.2) implies that the energy of a tree is a monotonically increasing function of any $m(T,k)$. In particular, if T' and T'' are two trees for which $m(T',k) \geq m(T'',k)$ holds for all $k \geq 1$, then $E(T') \geq E(T'')$. If, in addition, $m(T',k) > m(T'',k)$ for at least one k, then $E(T') > E(T'')$. Obviously, by Formula (1.3) and the monotonicity of the logarithm function, the result is also valid for ME. Thus, we can define a *quasi-order* "$\succeq$" as follows: If two graphs G_1 and G_2 have the same order and size, then

$$G_1 \succeq G_2 \Longleftrightarrow m(G_1,k) \geq m(G_2,k) \quad \text{for } 1 \leq k \leq \left\lfloor \frac{n}{2} \right\rfloor. \tag{1.4}$$

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. 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 $G_1 \# G_2$.

The relation $\sim$ is an equivalence relation in any set of graphs γ. The corresponding equivalence classes will be called *matching equivalence classes* (of the set γ). The relation $\succeq$ induces a partial ordering of the set $\gamma / \sim$. An equivalence class is said to be the *greatest* if it is greater than any of other class. A class is *maximal* if there is no other class greater than it. The graphs belonging to greatest (resp. maximal) matching equivalence classes will be said to be *m-greatest*(resp. *m-maximal*) in the set considered.

According to Eq.(1.3) and Eq.(1.4), we have

$$G_1 \succeq G_2 \Longrightarrow ME(G_1) \geq ME(G_2)$$

and

$$G_1 \succ G_2 \Longrightarrow ME(G_1) > ME(G_2).$$

It follows that the m-greatest graphs must have greatest matching energy, and the m-maximal graphs must have greater matching energy than other graphs not to be m-maximal.

A connected simple graph with n vertices and n, $(n+1)$, $(n+2)$ edges are called *unicyclic, bicyclic, tricyclic graphs*, respectively. Denote by $\mathscr{B}_n$ the set of all connected bicyclic graphs of order n, and by $\mathscr{T}_n$ the set of all connected tricyclic graphs on n vertices. Let S_n^* denote the graph obtained by joining one pendant vertex of S_n to its other two pendant vertices, respectively. Similarly, let S_n^{**} be the graph obtained by joining one pendent vertex of S_n to its another three pendent vertices, respectively. Let K_4^{n-4} denote the graph obtained by attaching $(n-4)$ pendent vertices to one of the four vertices of K_4. Of course, $S_n^{**}, K_4^{n-4} \in \mathscr{T}_n$ (as shown in Fig. 1.1). Denote by C_n the cycle graph of order n and P_n the path graph of order n, and let $P_n^{k,\ell}$ be the graph obtained by connecting two cycles C_k and C_ℓ with a path $P_{n-k-\ell}$.

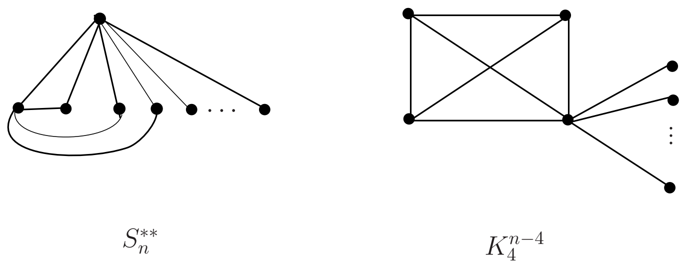

Figure 1.1: Tricyclic graphs with minimal matching energy.

As the research of extremal graph energy is an amusing work (for some newest literatures see [14–18, 22]), the study on extremal matching energy is also interesting.

In [13], 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, where S_n^+ is the graph obtained by adding a new edge to the star S_n. In [20], Ji et al. proved that for $G \in \mathscr{B}_n$ with $n \geq 10$ and $n = 8$, $ME(S_n^*) \leq ME(G) \leq ME(P_n^{4,n-4})$. In [19], the authors characterize the connected graphs (and bipartite graph) of order n having minimum matching energy with m $(n+2 \leq m \leq 2n-4)$ $(n \leq m \leq 2n-5)$ edges. Especially, among all tricyclic graphs of order $n \geq 5$, $ME(G) \geq ME(S_n^{**})$, with equality if and only if $G \cong S_n^{**}$ or $G \cong K_4^{n-4}$. For more results on the matching energy, we refer to [21, 23]. In this paper, we characterize the graphs with the maximal matching energy among all tricyclic graphs, and completely determine the tricyclic graphs with the maximal matching energy.

2 Main Results

In the 1980s, Gutman determined the unicyclic [6], bicyclic [7], tricyclic [9] graphs with maximal matchings, i.e., graphs that are extremal with regard to the quasi-ordering $\succeq$. We introduce the result on tricyclic graphs, which will be used in our proof.

Lemma 2.1 ([9]) *In the set of all tricyclic graphs with n vertices ($n \geq 4$) the greatest matching equivalence class exists only for $n = 4, 5, 6, 7, 8$ and 9. For $n \geq 10$ there exist two maximal matching equivalence classes. All these equivalence classes possess a unique element, except for $n = 9$, when the number of m-greatest graph is two. The corresponding graphs are presented in Fig. 2.2.*

Our results are obtained based on the result of Lemma 2.1.

Theorem 2.2 *Let $G \in \mathscr{T}_n$ with $n \geq 5$. Then for $n = 5$, $ME(G) \leq ME(G^5)$; for $n = 6$, $ME(G) \leq ME(G^6)$; for $n = 7$, $ME(G) \leq ME(G^7)$; for $n = 8$, $ME(G) \leq ME(G^8)$; for $n = 9$, $ME(G) \leq ME(G^9_{(1)}) = ME(G^9_{(2)})$; for $n = 10$, $ME(G) \leq ME(G^{10}_{(2)})$; for $n = 11$, $ME(G) \leq ME(G^{11}_{(2)})$; for $n = 12$, $ME(G) \leq ME(G^{12}_{(2)})$; for $n = 13$, $ME(G) \leq ME(G^{13}_{(2)})$; for $n \geq 14$, $ME(G) \leq ME(G^n_{(2)})$, with equality if and*

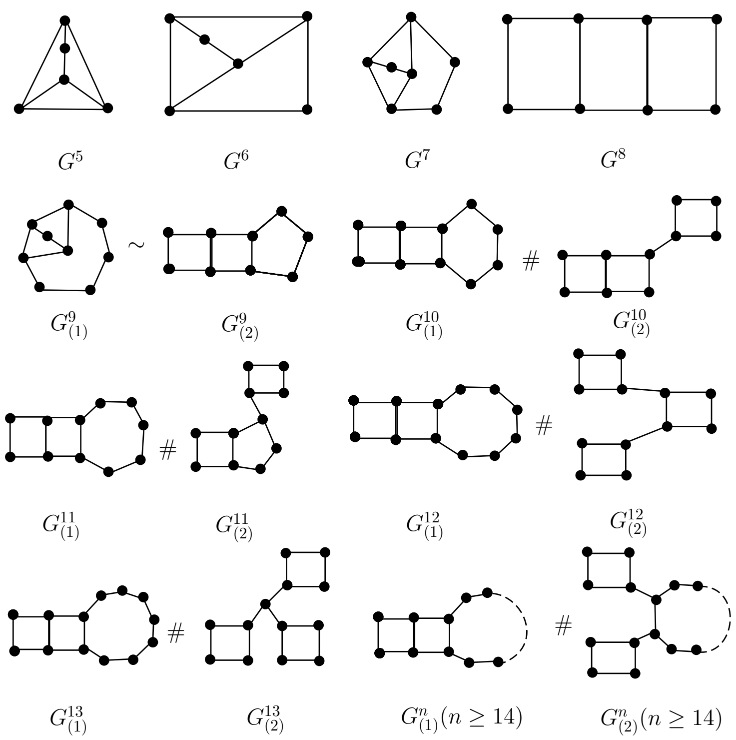

Figure 2.2: The tricyclic graphs with a maximal number of matchings.

only if $G \cong G^n_{(2)}$, *where* G^5, G^6, G^7, G^8, $G^9_{(1)}$, $G^9_{(2)}$, $G^{10}_{(2)}$, $G^{11}_{(2)}$, $G^{12}_{(2)}$, $G^{13}_{(2)}$, $G^n_{(2)}$ *are the graphs shown in Fig. 2.2.*

We will prove our theorem by using Coulson-type integral formula of matching energy Eq.(1.3), which is similar as the method to comparing the energies of two quasi-order incomparable graphs [14–18, 22]. The following lemmas are needed.

Lemma 2.3 ([25]) *For any real number* $X > -1$, *we have*

$$\frac{X}{1+X} \leq \ln(1+X) \leq X. \tag{2.1}$$

Let G be a simple graph. Let 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 such a result on the number of k-matchings of the graph $G(e/j)$.

Lemma 2.4 ([9]) *For all $j \geq 0$,*

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

We will divide Theorem 2.2 into the following two theorems according to the values of n.

Theorem 2.5 *Let $G \in \mathscr{T}_n$ with $n \geq 5$. Then:*
for $n=5$, $ME(G) \leq ME(G^5)$; for $n=6$, $ME(G) \leq ME(G^6)$; for $n=7$, $ME(G) \leq ME(G^7)$; for $n=8$, $ME(G) \leq ME(G^8)$; for $n=9$, $ME(G) \leq ME(G^9_{(1)}) = ME(G^9_{(2)})$; for $n=10$, $ME(G) \leq ME(G^{10}_{(2)})$; for $n=11$, $ME(G) \leq ME(G^{11}_{(2)})$; for $n=12$, $ME(G) \leq ME(G^{12}_{(2)})$; for $n=13$, $ME(G) \leq ME(G^{13}_{(2)})$, where G^5, G^6, G^7, G^8, $G^9_{(1)}$, $G^9_{(2)}$, $G^{10}_{(2)}$, $G^{11}_{(2)}$, $G^{12}_{(2)}$, $G^{13}_{(2)}$ are the graphs shown in Fig. 2.2. In each case, the equality holds if and only if G is isomorphic to the corresponding graph with maximal matching energy.

Proof. Let G be a graph in $\mathscr{T}_n$ with n vertices.

For $n = 5,6,7,8$, by Lemma 2.1, G^n is the m-greatest graph. We have known that the m-greatest graphs must have greatest matching energy. Hence if $G \ncong G^n$, then $ME(G) < ME(G^n)$.

When $n=9$, $G^9_{(1)}$ and $G^9_{(2)}$ are m-equivalent, that is, $m(G^9_{(1)},k) = m(G^9_{(2)},k)$ for all k. Then by Eq.(1.3), we have $ME(G^9_{(1)}) = ME(G^9_{(2)})$. Moreover, if $G \ncong G^9_{(1)}$ and $G \ncong G^9_{(2)}$, then $ME(G) < ME(G^9_{(1)}) = ME(G^9_{(2)})$ since $(G^9_{(1)} \sim G^9_{(2)}) \succ G$ by Lemma 2.1.

When $n=10$, both $G^{10}_{(1)}$ and $G^{10}_{(2)}$ are m-maximal. Thus, if $G \ncong G^{10}_{(1)}$ and $G \ncong G^{10}_{(2)}$, then $ME(G) < ME(G^{10}_{(1)})$ as well as $ME(G) < ME(G^{10}_{(2)})$. In addition, we have $m(G^{10}_{(1)},0) = 1$, $m(G^{10}_{(1)},1) = 12$, $m(G^{10}_{(1)},2) = 48$, $m(G^{10}_{(1)},3) = 76$, $m(G^{10}_{(1)},4) = 42$, $m(G^{10}_{(1)},5) = 5$ and $m(G^{10}_{(2)},0) = 1$, $m(G^{10}_{(2)},1) = 12$, $m(G^{10}_{(2)},2) = 48$, $m(G^{10}_{(2)},3) = 75$, $m(G^{10}_{(2)},4) = 42$, $m(G^{10}_{(2)},5) = 6$. Make use of Eq.(1.3), by computer-aided calculations, we get $ME(G^{10}_{(1)}) = 13.8644$ and $ME(G^{10}_{(2)}) = 13.9042$. Therefore, $ME(G) < ME(G^{10}_{(1)}) < ME(G^{10}_{(2)})$.

For $n = 11, 12, 13$, both $G^n_{(1)}$ and $G^n_{(2)}$ are m-maximal. Similarly, by the help of computer, we get $ME(G^{11}_{(1)}) = 14.9384$, $ME(G^{11}_{(2)}) = 14.9466$, $ME(G^{12}_{(1)}) = 16.3946$, $ME(G^{12}_{(2)}) = 16.5052$, $ME(G^{13}_{(1)}) = 17.5097$, $ME(G^{13}_{(2)}) = 17.5678$, respectively. Therefore, if $G \ncong G^n_{(2)}$, then we have $ME(G) \leq ME(G^n_{(1)}) < ME(G^n_{(2)})$.

The proof of the theorem is complete. ∎

Theorem 2.6 *Let $G \in \mathscr{T}_n$ with $n \geq 14$. Then $ME(G) \leq ME(G^n_{(2)})$, with equality if and only if $G \cong G^n_{(2)}$, where $G^n_{(2)}$ is the graph shown in Fig. 2.2.*

Proof. By Lemma 2.1, both $G^n_{(1)}$ and $G^n_{(2)}$ are m-maximal. The m-maximal graphs must have greater matching energy than other graphs not to be m-maximal. Thus, if $G \ncong G^n_{(1)}$ and $G \ncong G^n_{(2)}$, then $ME(G) < ME(G^n_{(1)})$ and $ME(G) < ME(G^n_{(2)})$. It is sufficient to show that $ME(G^n_{(1)}) < ME(G^n_{(2)})$. We will make full use of the definition of matching polynomial and Eq.(1.3).

Assume that $|G(e/j+2)| = n$, then$|G(e/j+1)| = n-1$ and $|G(e/j)| = n-2$. According to Lemma 2.4, we have

$$\begin{aligned}\alpha(G(e/j+2),x) &= \sum_{k\geq 0}(-1)^k m(G(e/j+2),k)x^{n-2k} \\ &= \sum_{k\geq 0}(-1)^k m(G(e/j+1),k)x^{n-2k} + \sum_{k\geq 0}(-1)^k m(G(e/j),k-1)x^{n-2k} \\ &= x\sum_{k\geq 0}(-1)^k m(G(e/j+1),k)x^{(n-1)-2k} \\ &- \sum_{k\geq 0}(-1)^{k-1} m(G(e/j),k-1)x^{(n-2)-2(k-1)} \\ &= x\alpha(G(e/j+1),x) - \alpha(G(e/j),x).\end{aligned}$$

By the definition of $G(e/j)$, clearly, $G^n_{(1)} = G_{(1)}(e/n-7)$ and $G^n_{(2)} = G_{(2)}(e/n-11)$, where $G_{(1)}$ and $G_{(2)}$ are the graphs shown in Fig. 2.3. Therefore, both $\alpha(G^n_{(1)}, x)$ and $\alpha(G^n_{(2)}, x)$ 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

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

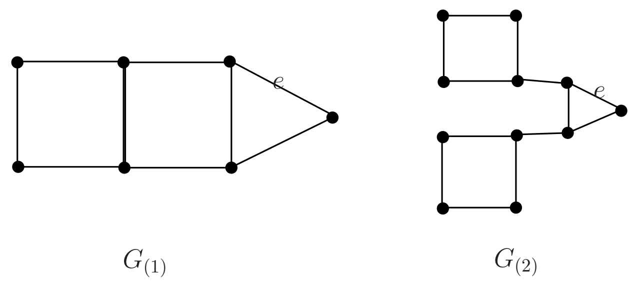

Figure 2.3: The fundamental graphs for constructing $G^n_{(1)}$ and $G^n_{(2)}$.

where $Y_1(x) = \frac{x+\sqrt{x^2-4}}{2}$, $Y_2(x) = \frac{x-\sqrt{x^2-4}}{2}$. By some elementary calculations, we can easily obtain the values of $C_i(x)$ $(i = 1, 2)$ as follows.

In the following, we first consider $\alpha(G^n_{(1)}, x)$. It is easy to calculate the number of k-matchings of $G_{(1)}$ and $G_{(1)}(e/1)$: $m(G_{(1)}, 0) = 1$, $m(G_{(1)}, 1) = 9$, $m(G_{(1)}, 2) = 21$, $m(G_{(1)}, 3) = 11$, $m(G_{(1)}, k) = 0$ for $k \geq 4$; $m(G_{(1)}(e/1), 0) = 1$, $m(G_{(1)}(e/1), 1) = 10$, $m(G_{(1)}(e/1), 2) = 29$, $m(G_{(1)}(e/1), 3) = 26$, $m(G_{(1)}(e/1), 4) = 5$, $m(G_{(1)}(e/1), k) = 0$ for $k \geq 5$. Then by Lemma 2.4, we can calculate the values of $m(G_{(1)}(e/j), k)$ for all $j \geq 2$ and $k \geq 0$. Thus, take the initial values as:

$$\begin{aligned}
\alpha(G_{(1)}(e/4), x) &= x^{11} - 13x^9 + 59x^7 - 114x^5 + 89x^3 - 21x \\
&= C_1(x)(Y_1(x))^{11} + C_2(x)(Y_2(x))^{11}; \\
\alpha(G_{(1)}(e/5), x) &= x^{12} - 14x^{10} + 71x^8 - 162x^6 + 165x^4 - 63x^2 + 5 \\
&= C_1(x)(Y_1(x))^{12} + C_2(x)(Y_2(x))^{12}.
\end{aligned}$$

It is easy to check that $Y_1(x) + Y_2(x) = x$ and $Y_1(x) \cdot Y_2(x) = 1$. Therefore, by solving the two equalities above, we get

$$C_1(x) = \frac{Y_1(x)\alpha(G_{(1)}(e/5), x) - \alpha(G_{(1)}(e/4), x)}{(Y_1(x))^{13} - (Y_1(x))^{11}}$$

and

$$C_2(x) = \frac{Y_2(x)\alpha(G_{(1)}(e/5), x) - \alpha(G_{(1)}(e/4), x)}{(Y_2(x))^{13} - (Y_2(x))^{11}}.$$

Define

$$A_1(x) = \frac{Y_1(x)\alpha(G_{(1)}(e/5), x) - \alpha(G_{(1)}(e/4), x)}{(Y_1(x))^{13} - (Y_1(x))^{11}}.$$

$$A_2(x) = \frac{Y_2(x)\alpha(G_{(1)}(e/5), x) - \alpha(G_{(1)}(e/4), x)}{(Y_2(x))^{13} - (Y_2(x))^{11}}.$$

Then we have $\alpha(G^n_{(1)}, x) = A_1(x)(Y_1(x))^n + A_2(x)(Y_2(x))^n$.

Now we consider $\alpha(G^n_{(2)}, x)$. Similarly, we get: $m(G_{(2)}, 0) = 1$, $m(G_{(2)}, 1) = 13$, $m(G_{(2)}, 2) = 59$, $m(G_{(2)}, 3) = 112$, $m(G_{(2)}, 4) = 84$, $m(G_{(2)}, 5) = 20$, $m(G_{(2)}, k) = 0$ for $k \geq 6$; $m(G_{(2)}(e/1), 0) = 1$, $m(G_{(2)}(e/1), 1) = 14$, $m(G_{(2)}(e/1), 2) = 71$, $m(G_{(2)}(e/1), 3) = 161$, $m(G_{(2)}(e/1), 4) = 164$, $m(G_{(2)}(e/1), 5) = 68$, $m(G_{(2)}(e/1), 6) = 8$, $m(G_{(2)}(e/1), k) = 0$ for $k \geq 7$. Then calculate the values of $m(G_{(2)}(e/j), k)$ for all $j \geq 2$ and $k \geq 0$ by using Lemma 2.4. We can then take the initial values as:

$$\begin{aligned}
\alpha(G_{(2)}, x) &= x^{11} - 13x^9 + 59x^7 - 112x^5 + 84x^3 - 20x \\
&= C_1(x)(Y_1(x))^{11} + C_2(x)(Y_2(x))^{11}; \\
\alpha(G_{(2)}(e/1), x) &= x^{12} - 14x^{10} + 71x^8 - 161x^6 + 164x^4 - 68x^2 + 8 \\
&= C_1(x)(Y_1(x))^{12} + C_2(x)(Y_2(x))^{12}.
\end{aligned}$$

Therefore, we obtain that:

$$C_1(x) = \frac{Y_1(x)\alpha(G_{(2)}(e/1), x) - \alpha(G_{(2)}, x)}{(Y_1(x))^{13} - (Y_1(x))^{11}}$$

and

$$C_2(x) = \frac{Y_2(x)\alpha(G_{(2)}(e/1), x) - \alpha(G_{(2)}, x)}{(Y_2(x))^{13} - (Y_2(x))^{11}}.$$

Define

$$B_1(x) = \frac{Y_1(x)\alpha(G_{(2)}(e/1), x) - \alpha(G_{(2)}, x)}{(Y_1(x))^{13} - (Y_1(x))^{11}}.$$

$$B_2(x) = \frac{Y_2(x)\alpha(G_{(2)}(e/1), x) - \alpha(G_{(2)}, x)}{(Y_2(x))^{13} - (Y_2(x))^{11}}.$$

Then we have $\alpha(G^n_{(2)}, x) = B_1(x)(Y_1(x))^n + B_2(x)(Y_2(x))^n$.

From the expression of $\alpha(G, x)$, we have

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

where $i^2 = -1$. Thus, by Eq.(1.3), we get

$$\begin{aligned}
ME(G^n_{(1)}) - ME(G^n_{(2)}) &= \frac{2}{\pi}\int_0^{\infty}\frac{1}{x^2}\ln\Big[\sum_{k\geq 0} m(G^n_{(1)},k)x^{2k}\Big]dx \\
&\quad - \frac{2}{\pi}\int_0^{\infty}\frac{1}{x^2}\ln\Big[\sum_{k\geq 0} m(G^n_{(2)},k)x^{2k}\Big]dx \\
&= \frac{2}{\pi}\int_0^{\infty}\frac{1}{x^2}\ln\frac{\sum_{k\geq 0} m(G^n_{(1)},k)x^{2k}}{\sum_{k\geq 0} m(G^n_{(2)},k)x^{2k}}dx \\
&= \frac{2}{\pi}\int_0^{\infty}\ln\frac{\sum_{k\geq 0} m(G^n_{(1)},k)x^{-2k}}{\sum_{k\geq 0} m(G^n_{(2)},k)x^{-2k}}dx \\
&= \frac{2}{\pi}\int_0^{\infty}\ln\frac{\alpha(G^n_{(1)},ix)}{\alpha(G^n_{(2)},ix)}dx \\
&= \frac{2}{\pi}\int_0^{\infty}\ln\frac{A_1(ix)(Y_1(ix))^n + A_2(ix)(Y_2(ix))^n}{B_1(ix)(Y_1(ix))^n + B_2(ix)(Y_2(ix))^n}dx.
\end{aligned} \tag{2.2}$$

By the definition of $Y_1(x)$ and $Y_2(x)$, we have $Y_1(ix) = \frac{x+\sqrt{x^2+4}}{2}i$ and $Y_2(ix) = \frac{x-\sqrt{x^2+4}}{2}i$. Now we define $Z_1(x) = -iY_1(x) = \frac{x+\sqrt{x^2+4}}{2}$, $Z_2(x) = -iY_2(x) = \frac{x-\sqrt{x^2+4}}{2}$, and

$$f_1 = i\alpha(G_{(1)}(e/4), ix) = x^{11} + 13x^9 + 59x^7 + 114x^5 + 89x^3 + 21x$$

$$f_2 = \alpha(G_{(1)}(e/5), ix) = x^{12} + 14x^{10} + 71x^8 + 162x^6 + 165x^4 + 63x^2 + 5$$

$$g_1 = i\alpha(G_{(2)}, ix) = x^{11} + 13x^9 + 59x^7 + 112x^5 + 84x^3 + 20x$$

$$g_2 = \alpha(G_{(2)}(e/1), ix) = x^{12} + 14x^{10} + 71x^8 + 161x^6 + 164x^4 + 68x^2 + 8.$$

Then we have $Y_1(ix) = iZ_1(x)$ and $Y_2(ix) = iZ_2(x)$. Moreover, It follows that

$$A_1(ix) = \frac{iZ_1(x)f_2 + if_1}{(iZ_1(x))^{13} - (iZ_1(x))^{11}} = \frac{Z_1(x)f_2 + f_1}{(Z_1(x))^{11}((Z_1(x))^2+1)}$$

$$A_2(ix) = \frac{iZ_2(x)f_2 + if_1}{(iZ_2(x))^{13} - (iZ_2(x))^{11}} = \frac{Z_2(x)f_2 + f_1}{(Z_2(x))^{11}((Z_2(x))^2+1)}$$

$$B_1(ix) = \frac{iZ_1(x)g_2 + ig_1}{(iZ_1(x))^{13} - (iZ_1(x))^{11}} = \frac{Z_1(x)g_2 + g_1}{(Z_1(x))^{11}((Z_1(x))^2+1)}$$

$$B_2(ix) = \frac{iZ_2(x)g_2 + ig_1}{(iZ_2(x))^{13} - (iZ_2(x))^{11}} = \frac{Z_2(x)g_2 + g_1}{(Z_2(x))^{11}((Z_2(x))^2+1)}.$$

Note that $Y_1(ix)\cdot Y_2(ix)=1$, $Z_1(x)\cdot Z_2(x)=-1$, $Z_1(x)+Z_2(x)=x$ and $Z_{1(x)}-Z_2(x)=\sqrt{x^2+4}$. We will distinguish with two cases.

Case 1. n is odd.

Now we have

$$\ln\frac{A_1(ix)(Y_1(ix))^{n+2}+A_2(ix)(Y_2(ix))^{n+2}}{B_1(ix)(Y_1(ix))^{n+2}+B_2(ix)(Y_2(ix))^{n+2}}-\ln\frac{A_1(ix)(Y_1(ix))^{n}+A_2(ix)(Y_2(ix))^{n}}{B_1(ix)(Y_1(ix))^{n}+B_2(ix)(Y_2(ix))^{n}}$$
$$=\ln\left(1+\frac{K_0(x)}{H_0(n,x)}\right),$$

where

$$K_0(x)=(A_1(ix)B_2(ix)-A_2(ix)B_1(ix))((Y_1(ix))^2-(Y_2(ix))^2)=(f_2g_1-f_1g_2)x$$
$$=-x^{18}-19x^{16}-146x^{14}-588x^{12}-1342x^{10}-1750x^8-1253x^6-460x^4-68x^2,$$

and

$$H_0(n,x)=(A_1(ix)(Y_1(ix))^n+A_2(ix)(Y_2(ix))^n)(B_1(ix)(Y_1(ix))^{n+2}+B_2(ix)(Y_2(ix))^{n+2})$$
$$=\alpha(G^n_{(1)},ix)\cdot\alpha(G^{n+2}_{(2)},ix)$$
$$=\left(i^n\sum_{k\geq 0}m(G^n_{(1)},k)x^{n-2k}\right)\left(i^{n+2}\sum_{k\geq 0}m(G^{n+2}_{(2)},k)x^{n+2-2k}\right)$$
$$=i^{2n+2}\left(\sum_{k\geq 0}m(G^n_{(1)},k)x^{n-2k}\right)\left(\sum_{k\geq 0}m(G^{n+2}_{(2)},k)x^{n+2-2k}\right).$$

Obviously, $K_0(x)<0$. Moreover, since n is odd, we have $i^{2n+2}=1$, it follows that $H_0(n,x)$ is a polynomial such that each term is of positive even degree of x and all coefficients are positive, i.e., $H_0(n,x)>0$. Hence, $\frac{K_0(x)}{H_0(n,x)}<0$, which deduces that $\ln(1+\frac{K_0(x)}{H_0(n,x)})<\ln 1=0$ for $x>0$ and odd n. So, the integrand of Eq.(2.2) is monotonically decreasing on n. Therefore, for $n\geq 14$,

$$\int_0^\infty\ln\frac{\alpha(G^n_{(1)},ix)}{\alpha(G^n_{(2)},ix)}dx\leq\int_0^\infty\ln\frac{\alpha(G^{15}_{(1)},ix)}{\alpha(G^{15}_{(2)},ix)}dx=\int_0^\infty\ln\frac{\alpha(G_{(1)}(e/8),ix)}{\alpha(G_{(2)}(e/4),ix)}dx.$$

By computer-aided calculations, we get $ME(G_{(1)}(e/8))=20.0728$ and $ME(G_{(2)}(e/4))=20.1086$. And then

$$\int_0^\infty\ln\frac{\alpha(G_{(1)}(e/8),ix)}{\alpha(G_{(2)}(e/4),ix)}dx=\frac{\pi}{2}\left(ME(G_{(1)}(e/8))-ME(G_{(2)}(e/4))\right)=-0.05639<0.$$

So $\int_0^\infty \ln \frac{\alpha(G^n_{(1)},ix)}{\alpha(G^n_{(2)},ix)}dx < 0$. That is,

$$ME(G^n_{(1)}) - ME(G^n_{(2)}) = \frac{2}{\pi}\int_0^\infty \ln \frac{\alpha(G^n_{(1)},ix)}{\alpha(G^n_{(2)},ix)}dx < 0.$$

Therefore, $ME(G^n_{(1)}) < ME(G^n_{(2)})$ when n is odd.

Case 2. n is even.

Since $x > 0$, when $n \longrightarrow \infty$, we have

$$\frac{A_1(ix)(Y_1(ix))^n + A_2(ix)(Y_2(ix))^n}{B_1(ix)(Y_1(ix))^n + B_2(ix)(Y_2(ix))^n} \longrightarrow \frac{A_1(ix)}{B_1(ix)}.$$

Then we have

$$\ln \frac{A_1(ix)(Y_1(ix))^n + A_2(ix)(Y_2(ix))^n}{B_1(ix)(Y_1(ix))^n + B_2(ix)(Y_2(ix))^n} - \ln \frac{A_1(ix)}{B_1(ix)} = \ln\left(1 + \frac{K_1(n,x)}{H_1(n,x)}\right),$$

where

$$\begin{aligned}K_1(n,x) &= A_2(ix)\cdot B_1(ix)\cdot (Y_2(ix))^n - A_1(ix)\cdot B_2(ix)\cdot (Y_2(ix))^n\\ &= \frac{(f_2g_1 - f_1g_2)(Z_2(x))^n}{\sqrt{x^2+4}}\cdot i^n\\ &= \frac{(-x^{17} - 19x^{15} - 146x^{13} - 588x^{11} - 1342x^9 - 1750x^7 - 1253x^5 - 460x^3 - 68x)}{\sqrt{x^2+4}}\\ &\quad \cdot (Z_2(x))^n \cdot i^n,\end{aligned}$$

and

$$\begin{aligned}H_1(n,x) &= A_1(ix)\cdot B_1(ix)\cdot (Y_1(ix))^n + A_1(ix)\cdot B_2(ix)\cdot (Y_2(ix))^n\\ &= A_1(ix)(B_1(ix)\cdot (Y_1(ix))^n + B_2(ix)\cdot (Y_2(ix))^n) = A_1(ix)\alpha(G^n_{(2)},ix)\\ &= i^n\cdot \frac{Z_1(x)f_2 + f_1}{(Z_1(x))^{11}((Z_1(x))^2+1)}\cdot \sum_{k\geq 0} m(G^n_{(2)},k)x^{n-2k}.\end{aligned}$$

Since n is even, $(Z_2(x))^n > 0$. Hence $K_1(n,x)/i^n$ is a polynomial of x with all coefficients being negative, namely, we always have $K_1(n,x)/i^n < 0$. On the other hand, since $x > 0$, we have $Z_1(x) = \frac{x+\sqrt{x^2+4}}{2} > 0$, $f_1 > 0$, $f_2 > 0$ and $m(G^n_{(2)},k) > 0$ for all $0 \leq k \leq \lfloor \frac{n}{2} \rfloor$. Hence $H_1(n,x)/i^n$ is a polynomial of x such that all the coefficients are positive. Therefore, $\frac{K_1(n,x)}{H_1(n,x)} < 0$ for all $x > 0$ and even n. Then $\ln(1+\frac{K_1(n,x)}{H_1(n,x)}) < \ln 1 = 0$, i.e.,

$$\ln \frac{A_1(ix)(Y_1(ix))^n + A_2(ix)(Y_2(ix))^n}{B_1(ix)(Y_1(ix))^n + B_2(ix)(Y_2(ix))^n} < \ln \frac{A_1(ix)}{B_1(ix)}.$$

Thus, we have proved that the integrand of Eq.(2.2) is less than the corresponding limit function when n is even. Furthermore, since

$$1+\frac{A_1(ix)-B_1(ix)}{B_1(ix)}=\frac{A_1(ix)}{B_1(ix)}=\frac{Z_1(x)f_2+f_1}{Z_1(x)g_2+g_1}>0,$$

we have $\frac{A_1(ix)-B_1(ix)}{B_1(ix)}>-1$. Then by Lemma 2.3, $\ln\frac{A_1(ix)}{B_1(ix)}\leq\frac{A_1(ix)-B_1(ix)}{B_1(ix)}$. By some computer-aided calculations, we obtain that $\int_0^\infty\frac{A_1(ix)-B_1(ix)}{B_1(ix)}dx=-0.09693$. It means that

$$\int_0^\infty \ln\frac{A_1(ix)}{B_1(ix)}dx\leq\int_0^\infty\frac{A_1(ix)-B_1(ix)}{B_1(ix)}dx<0.$$

Thus,

$$\begin{aligned}\frac{\pi}{2}(ME(G^n_{(1)})-ME(G^n_{(2)}))&=\int_0^\infty \ln\frac{A_1(ix)(Y_1(ix))^n+A_2(ix)(Y_2(ix))^n}{B_1(ix)(Y_1(ix))^n+B_2(ix)(Y_2(ix))^n}dx\\&<\int_0^\infty \ln\frac{A_1(ix)}{B_1(ix)}dx<0,\end{aligned}$$

i.e., $ME(G^n_{(1)})<ME(G^n_{(2)})$ when n is even.

Therefore, for all $n\geq 14$, we can always show that

$$ME(G^n_{(1)})<ME(G^n_{(2)}),$$

the proof is thus complete. ∎

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