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Ordering of Unicyclic Graphs with Perfect Matchings by Minimal Matching Energies

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Abstract

In 2012, Gutman and Wagner proposed the concept of the matching energy of a graph and pointed out that its chemical applications can go back to the 1970s. The matching energy of a graph is defined as the sum of the absolute values of the zeros of its matching polynomial. Let u and v be the non-isolated vertices of the graphs G and H with the same order, respectively. Let w_i be a non-isolated vertex of graph G_i where $i=1,2,\cdots,k$. We use $G_u(k)$ (respectively, $H_v(k)$) to denote the graph which is the coalescence of G (respectively, H) and $G_1,G_2,\cdots,G_k$ by identifying the vertices u (respectively, v) and $w_1,w_2,\cdots,w_k$. In this paper, we first present a new technique of directly comparing the matching energies of $G_u(k)$ and $H_v(k)$, which can tackle some quasi-order incomparable problems. As the applications of the technique, then we can determine the unicyclic graphs with perfect matchings of order $2n$ with the first to the ninth smallest matching energies for all $n \ge 211$.

Keywords

Matching Energy, Unicyclic Graph, Perfect Matching

1. Introduction

Let G be a simple and undirected graph with n vertices and $A(G)$ be its adjacency matrix. Let $\lambda_1,\lambda_2,\cdots,\lambda_n$ be the eigenvalues of $A(G)$. Then the energy of G, denoted by $E(G)$, is defined as [1]

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

A fundamental problem encountered within the study of graph energy is the characterization of the graphs that belong to a given class of graphs having maximal or minimal energy, for example, Trees with extremal energies [2]-[15]; Unicyclic graphs with extremal energies [16]-[21]; Bicyclic graphs with extremal energies [22] [23] [24] [25]; Tricyclic graphs with extremal energies [26] [27] [28]. For more details, they can be found in the recent book [29] and review [30].

A matching in a graph G is a set of pairwise nonadjacent edges. A matching is called k-matching if its size is k. Let $m(G,k)$ be the number of k-matching of G, where $m(G,k)=0$ for $k>\lfloor n/2 \rfloor$ or $k<0$. In addition, we assume that $m(G,0)=1$.

The matching polynomial of a graph G is defined as

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

Recently, Gutman and Wagner [31] generalized the concept of graph energy and defined the matching energy of a graph G based on the zeros of its matching polynomial.

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

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

Further, Gutman and Wagner [31] 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, in connection with the chemical applications of matching energy, for more details see [32] [33] [34].

Similar to the integral formula for the energy of graph, Gutman and Wagner [31] have shown a beautiful integral formula for the matching energy of a graph G as follows:

$$ME(G)=\frac{2}{\pi}\int_0^{+\infty}\frac{1}{x^2}\ln\left(\sum_{k=0}^{\lfloor n/2 \rfloor}m(G,k)x^{2k}\right)\mathrm{d}x. \tag{1}$$

Then $ME(G)$ is a strictly monotonically increasing function of those numbers $m(G,k)\left(k=0,1,\cdots,\lfloor n/2 \rfloor\right)$. In the followings, the method of the quasi-order relation "$\preceq$" is an important tool of comparing the matching energies of a pair of graphs.

Definition 1.2. *Let G_1 and G_2 be two graphs of order n. If $m(G_1,k)\le m(G_2,k)$ for all k with $1\le k\le\lfloor n/2 \rfloor$, then we write $G_1\preceq G_2$.*

Furthermore, if $G_1\preceq G_2$ and there exists at least one index j such that $m(G_1,j)<m(G_2,j)$, then we write $G_1\prec G_2$. If $m(G_1,k)=m(G_2,k)$ for all k, then we write $G_1\sim G_2$. According to the integral formula (1), we have for two graphs G_1 and G_2 of order n that

$$G_1 \preceq G_2 \Rightarrow ME(G_1) \le ME(G_2)$$
$$G_1 \prec G_2 \Rightarrow ME(G_1) < ME(G_2).$$

In [31], Gutman and Wagner shown that its matching energy coincides with its energy if T is a forest. Many properties of the matching energy are analogous to those of the graph energy. However, there are some notable differences. Then they raised a question: is it true that the matching energy of a graph G coincides with its energy if and only if G is a forest? Up to now, the question is still open.

The study on extremal matching energies is very interesting. In [31], Gutman and Wagner characterized the unicyclic graphs with the minimal and maximal matching energy. Zhu and Yang [35] determined the unicyclic graphs with the first eight minimal matching energies. In [36], Chen and Liu characterized the bipartite unicyclic graphs with the first $\lfloor (n-3)/4 \rfloor$ largest matching energies. Moreover, Chen *et al.* [37] determined the unicyclic odd-cycle graphs with the second to the fourth maximal matching energies. For bicyclic graph, Ji *et al.* [38] obtained the graphs with the minimal and maximal matching energy. In [39], Liu *et al.* further determined the bicyclic graphs with first five minimal matching energies and the second maximal matching energies, respectively. Chen and Shi [40] characterized tricyclic graph with maximal matching energy, for more results about extremal matching energies, see [41]-[47].

A fundamental problem encountered within the study of the matching energy is the characterization of the graphs that belong to a given class of graphs having maximal or minimal matching energy. One of the graph classes that are quite interestingly studied is the class of all unicyclic graphs with perfect matchings. As far as we are concerned, no results are on this topic. In this paper, we first present a new technique of directly comparing the matching energies of $G_u(k)$ and $H_v(k)$ in Section 2 (see **Figure 2**). As the applications of the technique, then we can determine the unicyclic graphs with perfect matchings of order $2n$ with the first to the ninth smallest matching energies for all $n \ge 211$ in Section 3.

For simplicity, if G_1 is isomorphic to G_2, then we write $G_1 = G_2$. If G_1 is not isomorphic to G_2, then we write $G_1 \ne G_2$. Let $\mathbb{A}(2n)$ be the set of the unicyclic graphs with perfect matchings of order $2n$. Let the unicyclic graphs A_1, A_2, A_3, A_4, A_4^*, A_5, A_6, A_7, A_8, A_9 be shown in **Figure 1**. The following theorem is the main result of this paper.

Theorem 1.1. *Let* $G \in \mathbb{A}(2n)$ *and* $n \ge 211$. *If* $G \ne A_1, A_2, A_3, A_4, A_4^*, A_5, A_6, A_7, A_8, A_9$, *then*

$$\begin{aligned} ME(A_1) &< ME(A_2) < ME(A_3) < ME(A_4) = ME(A_4^*) < ME(A_5) \\ &< ME(A_6) < ME(A_7) < ME(A_8) < ME(A_9) < ME(G) \end{aligned}.$$

2. A New Technique of Directly Comparing the Matching Energies of $G_u(k)$ and $H_v(k)$

By Definition 1.2, we can see that the quasi-order method can be used to compare the matching energies of two graphs. However, if the quantities $m(G,k)$ cannot be compared uniformly, then the common comparing method is invalid, and this happens quite often. Recently much effort has been made to tackle these quasi-order incomparable problems [35] [39] [40].

Let u and v be the non-isolated vertices of the graphs G and H with the same order, respectively. Let w_i be a non-isolated vertex of graph G_i where $i=1,2,\cdots,k$. We use $G_u(k)$ (respectively, $H_v(k)$) to denote the graph which is the coalescence of G (repectively, H) and $G_1,G_2,\cdots,G_k$ by identifying the vertices u (respectively, v) and $w_1,w_2,\cdots,w_k$ (see **Figure 2**). In [14], He *et al.* presented a new method of directly comparing the energies of the bipartite graphs $G_u(k)$ and $H_v(k)$. In this section, we apply the main idea of this method to present a new technique of comparing the matching energies of the graphs $G_u(k)$ and $H_v(k)$ which can be used to tackle these quasi-order incomparable problems.

In this paper, we assume that

$$\tilde{\alpha}(G)=\tilde{\alpha}(G,x)=\sum_{k=0}^{\lfloor n/2\rfloor} m(G,k)x^{n-2k}. \quad (2)$$

By Equation (2), we can immediately obtain the following results.

Lemma 2.1. *If two graphs G and H are disjoint, then*

$$\tilde{\alpha}(G\cup H)=\tilde{\alpha}(G)\cdot\tilde{\alpha}(H).$$

Lemma 2.2. ([35]) *Let* $G=(V(G),\mathcal{E}(G))$ *be a graph. If u is a vertex of G, then*

$$\tilde{\alpha}(G)=x\tilde{\alpha}(G-u)+\sum_{uv\in\mathcal{E}(G)}\tilde{\alpha}(G-u-v).$$

The coalescence of two graphs G and H with respect to vertex u in G and vertex v in H, denoted by $G_u\cdot H_v$ (sometimes abbreviated as $G\cdot H$), is the graph obtained by identifying the vertices u and v. Zhu and Yang [35] shown the recurrence relation of $\tilde{\alpha}(G\cdot H)$ in the following. For convenience of the reader, we present a full proof.

Lemma 2.3. ([35]) *Let* $G\cdot H$ *be the coalescence of two graphs G and H with respect to vertex u in G and vertex v in H. Then*

$$\tilde{\alpha}(G\cdot H)=\tilde{\alpha}(G)\tilde{\alpha}(H-v)+\tilde{\alpha}(G-u)\big(\tilde{\alpha}(H)-x\tilde{\alpha}(H-v)\big).$$

Proof. Using Lemmas 2.1 and 2.2, we can show

$$\begin{aligned}
\tilde{\alpha}(G\cdot H)&=x\tilde{\alpha}(G\cdot H-u)+\sum_{uw\in\mathcal{E}(G)}\tilde{\alpha}(G\cdot H-u-w)+\sum_{vt\in\mathcal{E}(H)}\tilde{\alpha}(G\cdot H-v-t)\\
&=x\tilde{\alpha}(G-u)\cdot\tilde{\alpha}(H-v)+\sum_{uw\in\mathcal{E}(G)}\tilde{\alpha}(G-u-w)\cdot\tilde{\alpha}(H-v)\\
&\quad+\sum_{vt\in\mathcal{E}(H)}\tilde{\alpha}(G-u)\cdot\tilde{\alpha}(H-v-t)\\
&=\left(x\tilde{\alpha}(G-u)+\sum_{uw\in\mathcal{E}(G)}\tilde{\alpha}(G-u-w)\right)\cdot\tilde{\alpha}(H-v)+\tilde{\alpha}(G-u)\cdot\sum_{vt\in\mathcal{E}(H)}\tilde{\alpha}(H-v-t)\\
&=\tilde{\alpha}(G)\cdot\tilde{\alpha}(H-v)+\tilde{\alpha}(G-u)\cdot\big(\tilde{\alpha}(H)-x\tilde{\alpha}(H-v)\big).
\end{aligned}$$

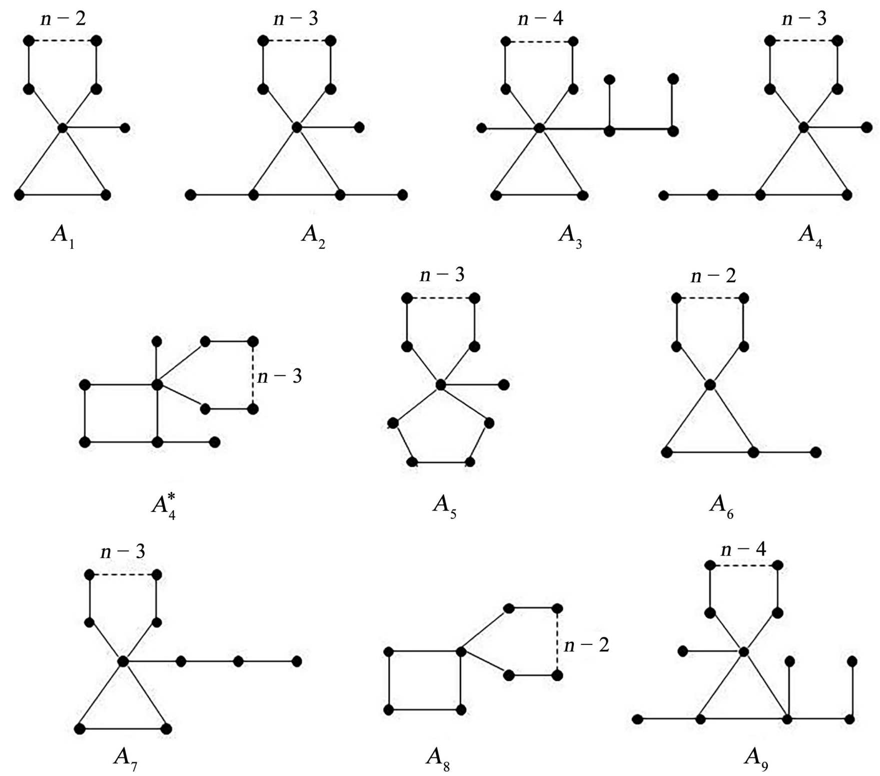

Figure 1. The graphs in $\mathbb{A}(2n)$ with the first to the ninth smallest matching energies. For each graph A_i, the dashed lines denote the copies of P_3 attached to the maximal degree vertex.

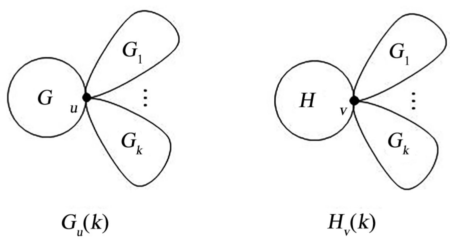

Figure 2. The graphs $G_u(k)$ and $H_v(k)$.

From Lemma 2.3, we can get the recurrence relations of the graphs $\tilde{\alpha}(G_u(k))$ and $\tilde{\alpha}(H_v(k))$ which is a generalization of the formula for $\tilde{\alpha}(G \cdot H)$.

Lemma 2.4. *Let* $G_u(k)$ *and* $H_v(k)$ *be defined as above* (*see* **Figure 2**). *Then we have the followings.*

1) $\tilde{\alpha}(G_u(k)) = \prod_{i=1}^{k} \tilde{\alpha}(G_i - w_i)\left(\tilde{\alpha}(G) + \tilde{\alpha}(G-u)\left(\sum_{i=1}^{k} \frac{\tilde{\alpha}(G_i)}{\tilde{\alpha}(G_i - w_i)} - kx\right)\right)$;

2) $\tilde{\alpha}(H_v(k)) = \prod_{i=1}^{k} \tilde{\alpha}(G_i - w_i)\left(\tilde{\alpha}(H) + \tilde{\alpha}(H-v)\left(\sum_{i=1}^{k} \frac{\tilde{\alpha}(G_i)}{\tilde{\alpha}(G_i - w_i)} - kx\right)\right)$.

Proof. 1) We prove the result by induction on *k*. When $k=1$, by Lemma 2.3 we have

$$\tilde{\alpha}(G_u(1)) = \tilde{\alpha}(G \cdot G_1) = \tilde{\alpha}(G)\tilde{\alpha}(G_1 - w_1) + \tilde{\alpha}(G-u)(\tilde{\alpha}(G_1) - x\tilde{\alpha}(G_1 - w_1)),$$

which implies that the result holds. We assume that the result holds for $k-1$ in what follows. For simplicity, we write $h_k = \sum_{i=1}^{k} \frac{\tilde{\alpha}(G_i)}{\tilde{\alpha}(G_i - w_i)} - kx$. By Lemmas 2.1 and 2.3, we can show

$$\begin{aligned}
\tilde{\alpha}(G_u(k)) &= \tilde{\alpha}(G_u(k-1) \cdot G_k) \\
&= \tilde{\alpha}(G_u(k-1))\tilde{\alpha}(G_k - w_k) + \tilde{\alpha}(G_u(k-1) - u)(\tilde{\alpha}(G_k) - x\tilde{\alpha}(G_k - w_k)) \\
&= \prod_{i=1}^{k-1} \tilde{\alpha}(G_i - w_i)(\tilde{\alpha}(G) + \tilde{\alpha}(G-u)h_{k-1})\tilde{\alpha}(G_k - w_k) \\
&\quad + \prod_{i=1}^{k-1} \tilde{\alpha}(G_i - w_i)\tilde{\alpha}(G-u)(\tilde{\alpha}(G_k) - x\tilde{\alpha}(G_k - w_k)) \\
&= \prod_{i=1}^{k-1} \tilde{\alpha}(G_i - w_i)((\tilde{\alpha}(G) + \tilde{\alpha}(G-u)h_{k-1})\tilde{\alpha}(G_k - w_k) \\
&\quad + \tilde{\alpha}(G-u)(\tilde{\alpha}(G_k) - \tilde{\alpha}(G_k - w_k))) \\
&= \prod_{i=1}^{k-1} \tilde{\alpha}(G_i - w_i)\tilde{\alpha}(G_k - w_k)\left(\tilde{\alpha}(G) + \tilde{\alpha}(G-u)h_{k-1} + \tilde{\alpha}(G-u)\left(\frac{\tilde{\alpha}(G_k)}{\tilde{\alpha}(G_k - w_k)} - x\right)\right) \\
&= \prod_{i=1}^{k} \tilde{\alpha}(G_i - w_i)\left(\tilde{\alpha}(G) + \tilde{\alpha}(G-u)h_{k-1} + \tilde{\alpha}(G-u)\left(\frac{\tilde{\alpha}(G_k)}{\tilde{\alpha}(G_k - w_k)} - x\right)\right) \\
&= \prod_{i=1}^{k} \tilde{\alpha}(G_i - w_i)\left(\tilde{\alpha}(G) + \tilde{\alpha}(G-u)\left(h_{k-1} + \frac{\tilde{\alpha}(G_k)}{\tilde{\alpha}(G_k - w_k)} - x\right)\right) \\
&= \prod_{i=1}^{k} \tilde{\alpha}(G_i - w_i)(\tilde{\alpha}(G) + \tilde{\alpha}(G-u)h_k)
\end{aligned}$$

Then we can see that the result holds.

2) The proof is similar to 1).

The following lemma illustrates an integral formula for the difference of the matching energies of two graphs with the same order which was obtained by Zhu and Yang [35].

Lemma 2.5. ([35]) *Let* $\alpha(G,x)$ *and* $\alpha(H,x)$ *be the matching polynomials of two graphs G and H with the same order, respectively. Then*

$$ME(G) - ME(H) = \frac{2}{\pi}\int_0^{+\infty} \ln \frac{\tilde{\alpha}(G,x)}{\tilde{\alpha}(H,x)} \mathrm{d}x.$$

Let $x > 0$. For simplicity, we write

$$h_k = \sum_{i=1}^{k} \frac{\tilde{\alpha}(G_i)}{\tilde{\alpha}(G_i - w_i)} - kx = \sum_{i=1}^{k} \frac{\tilde{\alpha}(G_i) - x\tilde{\alpha}(G_i - w_i)}{\tilde{\alpha}(G_i - w_i)}.$$

From Lemma 2.2, we have $h_k > 0$ and $h_l < h_k$ holds for any positive integer $l < k$.

In what follows, we define two sets M and M^c as follows:

$$M = \{x > 0 \mid \tilde{\alpha}(G-u)\tilde{\alpha}(H) - \tilde{\alpha}(G)\tilde{\alpha}(H-v) > 0\}$$

$$M^c = \{x > 0 \mid \tilde{\alpha}(G-u)\tilde{\alpha}(H) - \tilde{\alpha}(G)\tilde{\alpha}(H-v) \le 0\}.$$

It is easily checked that $M \cup M^c = (0, +\infty)$. Furthermore, we write

$$m_k(x) = \frac{\tilde{\alpha}(G) + h_k \tilde{\alpha}(G-u)}{\tilde{\alpha}(H) + h_k \tilde{\alpha}(H-v)}$$

$$m(x) = \frac{\tilde{\alpha}(G-u)}{\tilde{\alpha}(H-v)}.$$

Combining Lemma 2.4 with Lemma 2.5, we can present a new technique for directly comparing the matching energies of two graphs $G_u(k)$ and $H_v(k)$ in the following theorem.

Theorem 2.2. *Let M,* M^c, $m_k(x)$ *and* $m(x)$ *be defined as above. For all positive integers* $1 \le l < k$, *we have*

$$\int_M \ln m_l(x)\mathrm{d}x + \int_{M^c} \ln m(x)\mathrm{d}x \le \frac{\pi}{2}\left(ME(G_u(k)) - ME(H_v(k))\right)$$
$$\le \int_M \ln m(x)\mathrm{d}x + \int_{M^c} \ln m_l(x)\mathrm{d}x.$$

Proof. By some calculations, we can obtain that

$$m_k(x) - m_l(x) = \frac{\tilde{\alpha}(G) + h_k\tilde{\alpha}(G-u)}{\tilde{\alpha}(H) + h_k\tilde{\alpha}(H-v)} - \frac{\tilde{\alpha}(G) + h_l\tilde{\alpha}(G-u)}{\tilde{\alpha}(H) + h_l\tilde{\alpha}(H-v)}$$
$$= \frac{(h_k - h_l)\left(\tilde{\alpha}(G-u)\tilde{\alpha}(H) - \tilde{\alpha}(G)\tilde{\alpha}(H-v)\right)}{\left(\tilde{\alpha}(H) + h_k\tilde{\alpha}(H-v)\right)\left(\tilde{\alpha}(H) + h_l\tilde{\alpha}(H-v)\right)}.$$

$$m_k(x) - m(x) = \frac{\tilde{\alpha}(G) + h_k\tilde{\alpha}(G-u)}{\tilde{\alpha}(H) + h_k\tilde{\alpha}(H-v)} - \frac{\tilde{\alpha}(G-u)}{\tilde{\alpha}(H-v)}$$
$$= \frac{-\left(\tilde{\alpha}(G-u)\tilde{\alpha}(H) - \tilde{\alpha}(G)\tilde{\alpha}(H-v)\right)}{\left(\tilde{\alpha}(H) + h_k\tilde{\alpha}(H-v)\right)\tilde{\alpha}(H-v)}.$$

Thus, If $x \in M$, then $m_l(x) \le m_k(x) \le m(x)$. If $x \in M^c$, then $m(x) \le m_k(x) \le m_l(x)$.

Moreover, by Lemmas 2.4 and 2.5, we have

$$\frac{\pi}{2}\left(ME(G_u(k)) - ME(H_v(k))\right)$$
$$= \int_0^{+\infty} \ln m_k(x)\mathrm{d}x = \int_M \ln m_k(x)\mathrm{d}x + \int_{M^c} \ln m_k(x)\mathrm{d}x.$$

Then the result can be obtained immediately.

Next, we use the new technique to compare the matching energies of the quasi-order incomparable graphs A_5 and A_6, A_8 and A_9 (see **Figure 1**), respectively. Denote by C_k and P_k the cycle of length *k* and the path of length $k-1$, respectively.

Lemma 2.6. *If* $n \ge 6$, *then* $ME(A_5) < ME(A_6)$.

Proof. Let *G* be the graph obtained by attaching a pendent edge to a vertex *u* of C_5. Let *H* be the graph obtained by attaching a pendent edge and a pendent path of length 2 to the vertices *w* and *v* of C_3, respectively. Let $G_1 = G_2 = \cdots = G_{n-3} = P_3$ and w_i be the pendent vertex of G_i. Then

$G_u(n-3)=A_5$ and $H_v(n-3)=A_6$ (see **Figure 1**). By some calculations, we can show

$$\tilde{\alpha}(G)=x^6+6x^4+8x^2+1$$
$$\tilde{\alpha}(G-u)=x\left(x^4+3x^2+1\right)$$
$$\tilde{\alpha}(H)=x^6+6x^4+7x^2+1$$
$$\tilde{\alpha}(H-v)=\left(x^2+1\right)\left(x^3+2x\right).$$

It follows that

$$\tilde{\alpha}(G-u)\tilde{\alpha}(H)-\tilde{\alpha}(G)\tilde{\alpha}(H-v)=-2x^7-9x^5-9x^3-x.$$

This implies that $M=\varnothing$ and $M^c=(0,+\infty)$. By Theorem 2.2 and some calculations using the software MATLAB, we have

$$\begin{aligned}
&\frac{\pi}{2}\left(ME(A_5)-ME(A_6)\right)\\
&=\frac{\pi}{2}\left(ME\left(G_u(n-3)\right)-ME\left(H_v(n-3)\right)\right)\\
&\le\int_0^{+\infty}\ln m_3(x)\,\mathrm{d}x\\
&=\int_0^{+\infty}\ln\frac{\left(x^2+1\right)^2\left(x^8+10x^6+23x^4+12x^2+1\right)}{\left(x^2+1\right)^3\left(x^6+9x^4+13x^2+1\right)}\mathrm{d}x\\
&\doteq-0.0248<0.
\end{aligned}$$

Thus, $ME(A_5)<ME(A_6)$.

Lemma 2.7. *If* $n\ge 211$, *then* $ME(A_8)<ME(A_9)$.

Proof. Let G be the graph obtained by attaching two pendent paths of length 2 to the same vertex of C_4. Let H be the graph obtained by first attaching a pendent edge to each vertex of C_3 and then attaching a pendent path of length 2 to one vertex of C_3. Let u be the vertex of degree 4 in G and v be the vertex of degree 3 in H, respectively. Let $G_1=G_2=\cdots=G_{n-4}=P_3$ and w_i be the pendent vertex of G_i. Then $G_u(n-4)=A_8$ and $H_v(n-4)=A_9$ (see **Figure 1**). By some calculations, we can get the followings.

$$\tilde{\alpha}(G)=x^8+8x^6+17x^4+12x^2+2$$
$$\tilde{\alpha}(G-u)=\left(x^2+1\right)^2\left(x^3+2x\right)$$
$$\tilde{\alpha}(H)=x^8+8x^6+15x^4+8x^2+1$$
$$\tilde{\alpha}(H-v)=x\left(x^6+5x^4+5x^2+1\right),$$

which implies that

$$\tilde{\alpha}(G-u)\tilde{\alpha}(H)-\tilde{\alpha}(G)\tilde{\alpha}(H-v)=-x^3\left(x^2+1\right)^2\left(x^6+8x^4+11x^2+1\right).$$

It follows that $M=\varnothing$ and $M^c=(0,+\infty)$. By Theorem 2.2 and some calculations using the software MATLAB, we have

$$\begin{aligned}
&\frac{\pi}{2}\left(ME\left(A_8\right)-ME\left(A_9\right)\right)\\
&=\frac{\pi}{2}\left(ME\left(G_u\left(n-4\right)\right)-ME\left(H_v\left(n-4\right)\right)\right)\\
&\le\int_0^{+\infty}\ln m_{207}\left(x\right)\mathrm{d}x\\
&=\int_0^{+\infty}\ln\frac{\left(x^2+1\right)^{208}\left(x^6+214x^4+424x^2+2\right)}{\left(x^2+1\right)^{206}\left(x^{10}+216x^8+1055x^6+1055x^4+216x^2+1\right)}\mathrm{d}x\\
&\doteq -7.43\times10^{-5}<0.
\end{aligned}$$

Consequently, $ME\left(A_8\right)<ME\left(A_9\right)$.

3. Minimal Matching Energies of Unicyclic Graphs with Perfect Matchings of Order 2*n*

In this section, we will determine the unicyclic graphs with perfect matchings of order $2n$ with the first to the ninth smallest matching energies (*i.e.*, to prove Theorem 1.1).

In what follows, we denote by $M\left(G\right)$ a perfect matching of a graph G. Let $\hat{G}=G-M\left(G\right)-S_0$, where S_0 is the set of isolated vertices in $G-M\left(G\right)$. We call $\hat{G}$ the capped graph of G and G the original graph of $\hat{G}$. For example, the capped graphs of A_1,A_2,A_3,A_5 are shown in Figure 3.

Let $G\in\mathbb{A}\left(2n\right)$. Denote by $\mathcal{E}\left(G\right)$ the edge set of G. It is easy to see that $\mathcal{E}\left(G\right)=\mathcal{E}\left(\hat{G}\right)\cup M\left(G\right)$. Thus each k-matching Ω of G can be partitioned into two parts: $\Omega=\Phi\cup\Psi$, where $\Phi\subseteq\mathcal{E}\left(\hat{G}\right)$ and $\Psi\subseteq M\left(G\right)$. Let $r_j^{(2k)}\left(G\right)$ be the number of ways to choose k independent edges in G such that just j edges are in $\hat{G}$. We agree that $r_0^{(0)}\left(G\right)=1$ and $r_j^{(2k)}\left(G\right)=0\left(k<0\right)$. For example: $r_0^{(2k)}\left(G\right)=\binom{n}{k}$ and $r_1^{(2k)}\left(G\right)=n\binom{n-2}{k-1}$.

Then we have

$$m\left(G,k\right)=\sum_{j=0}^{k}r_j^{(2k)}\left(G\right)=p+\sum_{j=2}^{k}r_j^{(2k)}\left(G\right),\tag{3}$$

where

$$p=\binom{n}{k}+n\binom{n-2}{k-1}.$$

This is the main method to compute $m\left(G,k\right)$ of a graph G in what follows.

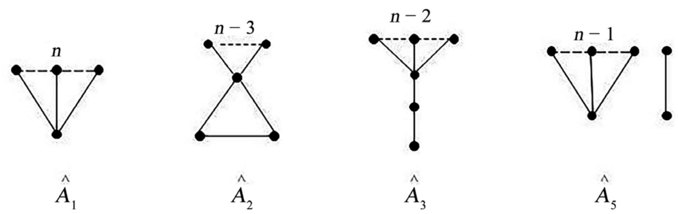

Figure 3. The capped graphs of A_1,A_2,A_3 and A_5. For each graph, the dashed lines denote the copies of P_2 attached to the maximal degree vertex.

Let X_n be the star of order *n*. Let Y_n be the graph of order *n* obtained by attaching $n-3$ pendent edges to a pendent vertex of P_3. Let Z_n be the graph of order *n* obtained from $P_4 = v_1v_2v_3v_4$ by attaching $n-5$ and one pendent edges to v_2 and v_3, respectively. In [2] and [31], the following results were shown.

Lemma 3.1. ([2]) *Let T be a tree of order* $n \geq 5$. *Then* $m(X_n,k) \leq m(Y_n,k) \leq m(Z_n,k) \leq m(T,k)$, *and the equalities do not hold for all k, where* $T \neq X_n, Y_n, Z_n$ *and* $0 \leq k \leq \lfloor n/2 \rfloor$.

Lemma 3.2. ([31]) *Suppose that G is a connected graph and T is 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 quasi-order decreases (unless T is already such a star).*

Let S_n^l be the unicyclic graph of order *n* obtained by attaching $n-l$ pendent edges to one vertex of C_l.

Lemma 3.3. ([43]) *Let G be a unicyclic graph of order n with a cycle of length l. If* $G \neq S_n^l$, *then* $G \succ S_n^l$.

Let R_n^3 be the graph of order *n* obtained by attaching $n-4$ and one pendent edges to v_1 and v_2 of $C_3 = v_1v_2v_3v_1$, respectively. Let $C_3(a,b,c)$ be the unicyclic graph obtained by attaching a,b,c pendent edges to v_1,v_2,v_3 of $C_3 = v_1v_2v_3v_1$, respectively. Let Q_n^3 be the graph of order *n* obtained by attaching $n-4$ pendent edges to the pendent vertex of $C_3(1,0,0)$. The graphs S_n^3, R_n^3 and Q_n^3 are shown in **Figure 4**.

Lemma 3.4. *Let G be a unicyclic graph of order* $n \geq 9$. *If* $G \neq S_n^3, R_n^3$, *then* $m(G,2) \geq 2n-6$.

Proof. Let *G* be a unicyclic graph with the unique cycle of length *l*. We consider the following cases.

Case 1: $l \geq 5$.

By Lemma 3.10, we have $G \succeq S_n^l$. Then

$m(G,2) \geq m(S_n^l,2) \geq (n-l)(l-2) \geq 3(n-5) \geq 2n-6$.

Case 2: $l = 4$.

Using Lemma 3.10, we can show $G \succeq S_n^4$. So, $m(G,2) \geq m(S_n^4,2) = 2n-6$.

Case 3: $l = 3$.

Denote by $d_G(u)$ the degree of the vertex *u* in *G*. Let $C_3 = v_1v_2v_3v_1$ be the unique cycle of the unicyclic graph *G* and $N(G) = \{v_i \mid d_G(v_i) \geq 3, i = 1,2,3\}$.

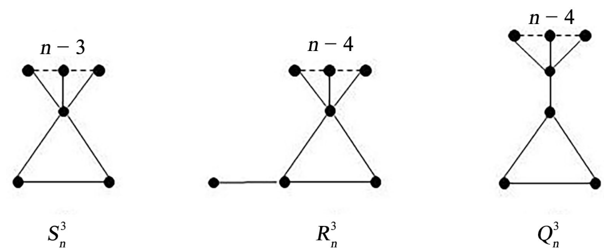

Figure 4. The graphs S_n^3, R_n^3 and Q_n^3 in Lemma 3.4. For each graph, the dashed lines denote the copies of P_2 attached to the maximal degree vertex.

Subcase 3.1: $|N(G)|=1$.

Without loss of generality, we can assume that $d_G(v_1)\ge 3$. Let T be the rooted tree of order $n-2$ with the root v_1 in *G*. If $T=X_{n-2}$, then $G=Q_n^3$ ($G\ne S_n^3$). Then $m(G,2)=3n-11>2n-6$. If $T=Y_{n-2}$, then
$m(G,2)\ge(n-3)+m(Y_{n-2},2)+2=(n-3)+(n-5)+2=2n-6$. If $T\ne X_{n-2},Y_{n-2}$, then by Lemma 3.8 we have

$$m(G,2)\ge(n-3)+m(T,2)\ge(n-3)+m(Z_{n-2},2)=n-3+2(n-6)=3n-15\ge 2n-6.$$

Subcase 3.2: $|N(G)|=2$.

Without loss of generality, we can assume that $d_G(v_1)\ge 3$ and $d_G(v_2)\ge 3$. Let T_1 and T_2 be the rooted tree with the root v_1 and v_2 in *G*, respectively.

If $T_1=P_2$ or $T_2=P_2$, then by Lemma 3.9 we can show $m(G,2)\ge m(R_n^3,2)=2n-7$. Since $G\ne R_n^3$, we have $m(G,2)\ge 2n-6$.

If $T_1\ne P_2$ and $T_2\ne P_2$, then by Lemma 3.9 we have $G\succeq C_3(a,b,0)$ ($a+b=n-3$). Thus, $m(G,2)\ge m(C_3(a,b,0),2)\ge a+b+ab\ge n-3+2(n-5)=3n-13>2n-6$.

Subcase 3.3: $|N(G)|=3$.

According to Lemma 3.9, we have $G\succeq C_3(a,b,c)$ ($a+b+c=n-3$). Then we have

$$\begin{aligned} m(G,2) &\ge a+b+c+ab+bc+ac \\ &\ge n-3+a+b-1+b+c-1+a+c-1 \\ &= n-3+2(n-3)-3 \\ &= 3n-12>2n-6. \end{aligned}$$

Thus we have completed the proof.

Lemma 3.5. *Let* $G\in\mathbb{A}(2n)$ *and* $n\ge 9$. *If* $G\ne A_1,A_2,A_3,A_4,A_4^*,A_5,A_6,A_7,A_8,A_9$, *then* $m(\hat{G},2)\ge 2n-6$.

Proof. We consider the following cases.

Case 1: $\hat{G}$ is a connected graph.

Subcase 1.1: $\hat{G}$ is a tree.

It can easily be verified that $G=A_1$ as $\hat{G}=X_{n+1}$ and $G=A_3,A_4,A_4^*,A_6$ as $\hat{G}=Y_{n+1}$. Thus, $\hat{G}\ne X_{n+1},Y_{n+1}$. By Lemma 3.8, we have $m(\hat{G},2)\ge m(Z_{n+1},2)=2n-6$.

Subcase 1.2: $\hat{G}$ is a connected unicyclic graph.

It can be shown that $G=A_2$ as $\hat{G}=S_n^3$ and $G=A_9$ as $\hat{G}=R_n^3$. Therefore, $\hat{G}\ne S_n^3,R_n^3$. According to Lemma 3.11, we have $m(\hat{G},2)\ge 2n-6$.

Case 2: $\hat{G}$ is a unconnected graph.

Subcase 2.1: $\hat{G}$ is only composed of trees.

It can be checked that $G=A_5,A_7,A_8$ as $\hat{G}=X_n\cup P_2$. Then, $\hat{G}\ne X_n\cup P_2$. Let $\hat{G}_1$ be the coalescence of all trees in a way such that $\hat{G}_1\ne X_{n+1},Y_{n+1}$. It is clear that $m(\hat{G},2)>m(\hat{G}_1,2)$. Similar to Subcase 1.1, we have $m(\hat{G},2)>2n-6$.

Subcase 2.2: $\hat{G}$ is composed of trees and unicyclic graphs.

Let $\hat{G}_2$ be the coalescence of all trees and unicyclic graphs in a way such that $\hat{G}_2\ne S_n^3,R_n^3$. It is obvious that $m(\hat{G},2)>m(\hat{G}_2,2)$. Similar to Subcase 1.2, we have $m\left(\hat{G},2\right)>2n-6$.

Then we have completed the proof.

From Lemma 3.5, we can immediately derive the following result.

Lemma 3.6. *Let* $G\in\mathbb{A}(2n)$ *and* $n\geq 9$. *If* $G\neq A_1,A_2,A_3,A_4,A_4^*,A_5,A_6,A_7,A_8,A_9$, *then* $G\succ A_9$.

Proof. By Equation (3) and Lemma 3.12, when $k\geq 2$, we can get

$$\begin{aligned} m(G,k) &= p+\sum_{j=2}^{k} r_j^{(2k)}(G) \geq p+r_2^{(2k)}(G) \\ &\geq p+m\left(\hat{G},2\right)\binom{n-4}{k-2} \geq p+(2n-6)\binom{n-4}{k-2}. \end{aligned}$$

Furthermore, by some calculations we have

$$m(A_9,k)=p+(2n-7)\binom{n-4}{k-2}.$$

Then we can see that $G\succ A_9$.

Combining Lemma 2.6 with Lemma 2.7, we can show the followings.

Lemma 3.7. *If* $n\geq 211$, *then*

$$\begin{aligned} &ME(A_1)<ME(A_2)<ME(A_3)<ME(A_4)=ME(A_4^*)<ME(A_5) \\ &\quad <ME(A_6)<ME(A_7)<ME(A_8)<ME(A_9) \end{aligned}.$$

Proof. Using Equation (4) and some calculations, we can get

$$m(A_1,k)=p$$

$$m(A_2,k)=p+(n-3)\binom{n-4}{k-2}$$

$$m(A_3,k)=p+(n-2)\binom{n-4}{k-2}$$

$$m(A_4,k)=p+\binom{n-3}{k-2}+(n-3)\binom{n-4}{k-2}$$

$$m(A_4^*,k)=p+\binom{n-3}{k-2}+(n-3)\binom{n-4}{k-2}$$

$$m(A_5,k)=p+2\binom{n-3}{k-2}+(n-3)\binom{n-4}{k-2}$$

$$m(A_6,k)=p+(n-3)\binom{n-3}{k-2}$$

$$m(A_7,k)=p+(n-1)\binom{n-3}{k-2}$$

$$m(A_8,k)=p+\binom{n-2}{k-2}+(n-2)\binom{n-3}{k-2}$$

$$m(A_9,k)=p+(2n-7)\binom{n-4}{k-2}.$$

It implies that $A_1 \prec A_2 \prec A_3 \prec A_4 \prec A_5$ and $A_6 \prec A_7 \prec A_8$. From Lemmas 2.6 and 2.7, the result can be easily obtained.

Proof of Theorem 1.1:

Proof. The result can follow immediately by Lemmas 3.13 and 3.14.

4. Conclusions

In this paper, we first present a new technique of directly comparing the matching energies of $G_u(k)$ and $H_v(k)$, which can tackle some quasi-order incomparable problems. As the applications of the technique, we then determine the unicyclic graphs with perfect matchings of order $2n$ with the first to the ninth smallest matching energies for all $n \geq 211$. Furthermore, we can consider characterizing the extremal graphs with maximal or minimal matching energy for other classes of graphs, e.g. graphs with different parameters. These are our work in the future.

The results presented in this paper are for a fixed graph. In reality, most of the graphs or networks are evolving. Some graph invariants have been studied in this setting, e.g. the Estrada index of evolving graphs [48]; Laplacian Estrada and normalized Laplacian Estrada indices of evolving graphs [49]. Then we can consider studying the matching energy of evolving graphs in the future.

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Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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