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EXTREMAL SKEW ENERGY OF DIGRAPHS WITH NO EVEN CYCLES

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Abstract. Let D be a digraph with skew-adjacency matrix $S(D)$. Then the skew energy of D is defined as the sum of the norms of all eigenvalues of $S(D)$. Denote by $\mathcal{O}_n$ the class of digraphs of order n with no even cycles, and by $\mathcal{O}_{n,m}$ the class of digraphs in $\mathcal{O}_n$ with m arcs. In this paper, we first give the minimal skew energy digraphs in $\mathcal{O}_n$ and $\mathcal{O}_{n,m}$ with $n-1 \le m \le \frac{3}{2}(n-1)$. Then we determine the maximal skew energy digraphs in $\mathcal{O}_{n,n}$ and $\mathcal{O}_{n,n+1}$, and in the latter case we assume that n is even.

1. **Introduction**

Let D be a digraph with vertex set $V(D) = \{v_1, v_2, \dots, v_n\}$ and arc set $\Gamma(D)$. Denote by $v(D)$ and $\gamma(D)$ the numbers of vertices and arcs of the digraph D, respectively. Throughout this paper, we always assume that D has no loops or multiple arcs or directed cycles of length 2, thus the underlying graph $\overline{D}$ of D is simple. In other words, D is an orientation of a simple undirected graph. *The skew-adjacency matrix* [1] of D is the $n \times n$ matrix $S(D) = [s_{ij}]$, where $s_{ij} = 1$ if $(v_i, v_j) \in \Gamma(D)$, $s_{ij} = -1$ if $(v_j, v_i) \in \Gamma(D)$, and $s_{ij} = 0$ otherwise. The characteristic polynomial of $S(D)$, which is called *the skew characteristic polynomial* of D, has the form

$$\phi_s(D, \lambda) = \sum_{k=0}^{n} a_k(D)\lambda^{n-k}.$$

Let $\{\lambda_1, \lambda_2, \dots, \lambda_n\}$ be the eigenvalues of $S(D)$, which are just the roots of the equation $\phi_s(D, \lambda) = 0$. Obviously, they are all pure imaginary numbers. *The skew energy* [1] of D, denoted by $\mathcal{E}_s(D)$, is defined as the sum of the norms of them, i.e.,

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

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For convenience, when we say walks, paths, cycles, degrees, matchings, etc. of a digraph, we mean the same as those they are in its underlying graph, unless otherwise stated.

The concept of energy of a simple undirected graph was introduced by Gutman in [6], which has a close link to chemistry and has been extensively studied. We refer the book [14] and a survey [7] to the reader for details. There are situations when chemists use digraphs rather than graphs. One such situation is when vertices represent distinct chemical species and arcs represent the direction in which a particular reaction takes place between the two corresponding species. So it is hoped that the skew energy will have similar applications as energy in chemistry.

Since Adiga, Balakrishnan and So in [1] proposed the concept of skew energy, many results have been obtained, most of which are collected in a recent survey [13]. One of the fundamental questions that is encountered in the study of skew energy is which digraphs in a given class attain extremal skew energy. Such results have been obtained for directed trees, unicyclic and bicyclic digraphs [1, 10, 15]. All 1-, 2-, 3- and 4-regular graphs were characterized which have orientations such that the resultant oriented graphs attain maximum skew energy [1, 2, 4, 5]. Moreover, from Pfaffian theory (See Remark 2.3), it can be found that the coefficients of skew characteristic polynomials of digraphs with no even cycles have special forms, which motivates us to consider extremal skew energy of the digraphs with no even cycles.

Let $\mathcal{O}_n$ be the class of digraphs of order n with no even cycles, and $\mathcal{O}_{n,m}$ be the class of digraphs in $\mathcal{O}_n$ with m arcs. For any digraph $D \in \mathcal{O}_{n,m}$, since there are no even cycles in it, any two cycles in D have at most one common vertex. So we have $n-1 \leq m \leq \frac{3}{2}(n-1)$. In this paper, we first give some definitions and deduce some basic results in Section 2. Then in Section 3, we give the minimal skew energy digraphs in $\mathcal{O}_n$ and $\mathcal{O}_{n,m}$ with $n-1 \leq m \leq \frac{3}{2}(n-1)$. In Sections 4 and 5, we, respectively, determine the maximal skew energy digraphs in $\mathcal{O}_{n,n}$ and $\mathcal{O}_{n,n+1}$, and in the latter case we assume that n is even.

2. Preliminaries

We first give some basic definitions. An r-matching in a graph D is a subset of r edges such that every vertex of $V(D)$ is incident with at most one edge in it. Denote by $m(D,r)$ the number of all r-matchings in D and set $m(D,0)=1$. The matching polynomial of D is defined as

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

For convenience, we use the so-called signless matching polynomial [11] here as for undirected graphs,

$$m^+(D,x) = \sum_{k=0}^{\lfloor n/2 \rfloor} m(D,k) x^{2k}. \tag{2.1}$$

A digraph H is called a "basic digraph" if each component of H is a K_2 or a cycle with even length (or even cycle). An even cycle C in a digraph D is called evenly directed if for either choice of direction of traversal around C, the number of edges of C directed in the direction of the traversal is even. Otherwise, such an even cycle is called oddly directed. Just like the Sachs Theorem for undirected graph, Gong et al. [3] gave an important property about the coefficients of the skew characteristic polynomial of a digraph.

Lemma 2.1. *Let D be an unweighted digraph on n vertices with the skew characteristic polynomial*

$$\phi_s(D,\lambda)=\sum_{i=0}^{n}(-1)^i a_i\lambda^{n-i}=\lambda^n-a_1\lambda^{n-1}+a_2\lambda^{n-2}+\cdots+(-1)^{n-1}a_{n-1}\lambda+(-1)^n a_n.$$

Then $a_i=0$ if i is odd, and

$$a_i=\sum_{\mathcal{H}}(-1)^{c^+}2^c \quad \text{if } i \text{ is even},$$

where the summation is over all basic directed subgraphs $\mathcal{H}$ of D having i vertices and c^+, c are respectively the number of evenly directed even cycles and even cycles contained in $\mathcal{H}$.

From this lemma, we find that the direction of an odd cycle has no effect on the coefficients of the skew characteristic polynomial. Then for the skew characteristic polynomial of a digraph $D\in\mathcal{O}_n$, if i is odd, $a_i=0$; if i is even, a_i only has a relevance to K_2, which bears on the matching number of D. We can get the following corollary immediately.

Corollary 2.2. *Let D be a digraph in $\mathcal{O}_n$. Then its skew characteristic polynomial is of the form*

$$\phi_s(D,\lambda)=\sum_{i=0}^{\lfloor n/2\rfloor}m(D,i)\lambda^{n-2i},$$

Remark 2.3. *The above result can be also deduced from the Pfaffian theory* [16]*. Recall that a Pfaffian orientation of G is such an orientation for the edges of G under which every even cycle C of G such that $G\setminus V(C)$ has a perfect matching has the property that there are odd number of edges directed in either direction of the cycle C. Suppose that G has a Pfaffian orientation D with skew-adjacency matrix $S(D)$. Then the determinant of $S(D)$ equals the square of the number of perfect matchings of G, i.e., $\det(S(D))=m^2(G,n/2)$. Moreover, if G contains no even cycles, then any orientation D of G is a Pfaffian orientation of G. Now $\det(S(D))=m^2(G,n/2)=0$ or 1, since two distinct perfect matchings contain an even cycle. Next we consider the coefficients of the skew characteristic polynomial of D. Let D_k be a subgraph of D on k vertices with skew-adjacency matrix S_k. Then*

$$(-1)^k a_k(D)=\sum_{D_k}\det(S_k)=\sum_{D_k}m^2(D_k,k/2).$$

Obviously, if k is odd, then $a_k(D)=0$; otherwise, $a_k(D)=m(D,k/2)$.

Therefore, in the class $\mathcal{O}_n$ the skew characteristic polynomial of a digraph is independent of its directions, so is the skew energy. Then throughout this paper we can consider digraphs with arbitrary directions. Since $a_{2k}(D)=m(D,k)$, we get the next result.

Lemma 2.4. *Let D_1 and D_2 be two vertex-disjoint digraphs. Then*

$$a_{2k}(D_1 \cup D_2) = \sum_{i=0}^{i=k} a_{2i}(D_1) \cdot a_{2k-2i}(D_2).$$

The next property is given in [9].

Lemma 2.5. *Let D be a digraph, and let $e = (u, v)$ be an edge of D that is not on any even cycles of D. Then*

$$a_{2k}(D) = a_{2k}(D - e) + a_{2k-2}(D - u - v).$$

Furthermore, if $e = (u, v)$ is a pendant edge with the pendant vertex v. Then

$$a_{2k}(D) = a_{2k}(D - v) + a_{2k-2}(D - u - v).$$

In [10], Hou et al. obtained the following integral formula for the skew energy.

Lemma 2.6. *Let D be a digraph in $\mathcal{O}_n$. Then*

$$\mathcal{E}_s(D) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \log(1 + \sum_{i=1}^{\lfloor \frac{n}{2} \rfloor} a_{2i} x^{2i}) dx.$$

From Lemma 2.6, $\mathcal{E}_s(D)$ is an increasing function in $a_{2i}(D)$, $0 \le i \le \lfloor \frac{n}{2} \rfloor$. Consequently, for two digraphs $D_1, D_2 \in \mathcal{O}_n$, if $a_{2i}(D_1) \ge a_{2i}(D_2)$ for all $0 \le i \le \lfloor \frac{n}{2} \rfloor$, then $\mathcal{E}_s(D_1) \ge \mathcal{E}_s(D_2)$. If at least one of the inequalities $a_{2i}(D_1) \ge a_{2i}(D_2)$ is strict, then we have $\mathcal{E}_s(D_1) > \mathcal{E}_s(D_2)$.

By Corollary 2.2, Lemma 2.6 and Eq. (2.1), we have

$$\mathcal{E}_s(D) = \frac{2}{\pi} \int_{0}^{+\infty} \frac{1}{x^2} \log m^+(D, x) dx. \tag{2.2}$$

Now we list some useful properties of the signless matching polynomial $m^+(D, x)$, which is valid for digraphs as well as undirected graphs, and already appeared in [12].

Lemma 2.7. *Let D_1 and D_2 be two vertex-disjoint graphs. Then*

$$m^+(D_1 \cup D_2, x) = m^+(D_1, x) \cdot m^+(D_2, x).$$

Lemma 2.8. *Let $e = uv$ be an edge of a graph D. Then we have*

$$m^+(D, x) = m^+(D - e, x) + x^2 m^+(D - u - v, x).$$

Lemma 2.9. *Let P_t denote a path on t vertices. Then*

$$m^+(P_t, x) = m^+(P_{t-1}, x) + x^2 m^+(P_{t-2}, x), \text{ for any } t \ge 1.$$

The initials are $m^+(P_0, x) = m^+(P_1, x) = 1$, and we define $m^+(P_{-1}, x) = 0$.

We end this section with some notations. Denote by P_n, C_n, S_n the directed path, cycle, star of order n with arbitrary directions, P_n^{ℓ} the unicyclic digraph obtained by connecting a vertex of C_ℓ with a leaf of $P_{n-\ell}$, and $P_n^{\ell,s}$ the digraph obtained from two cycles C_ℓ and C_s joined by a path $P_{n-\ell-s+2}$. Let $S_{n,m} \in \mathcal{O}_{n,m}$, $n - 1 \le m \le n - 1 + \lfloor \frac{n-1}{2} \rfloor$, be the digraph obtained from S_n by attaching $m - n + 1$

edges to different pairs of pendant vertices, such that the pendant vertices of S_n is of degree no more than 2 in the digraph $S_{n,m}$. Clearly, $S_{n,n-1} \cong S_n$. We give the following underlying undirected graph of $S_{n,n+2}$ for example.

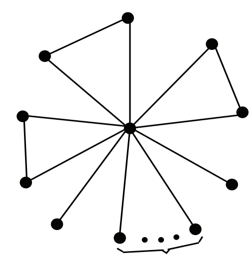

FIGURE 1. The underlying undirected graph of $S_{n,n+2}$.

3. Minimal skew energy digraphs with no even cycles

For directed trees, the skew energy has the following property [1].

Lemma 3.1. *The skew energy of a directed tree is the same as the energy of its underlying tree.*

Corollary 3.2. *For all trees in $\mathcal{O}_{n,n-1}$, the directed star S_n has the minimal skew energy.*

Now we can get the next two theorems.

Theorem 3.3. *Let D be a connected digraph in $\mathcal{O}_n$. If $D \ncong S_n$, then $\mathcal{E}_s(D) > \mathcal{E}_s(S_n)$.*

Proof. By Lemma 2.5,

$$a_{2k}(D,x) = a_{2k}(D-e,x) + a_{2k-2}(D-u-v,x) \geq a_{2k}(D-e,x).$$

Thus $\mathcal{E}_s(D) \geq \mathcal{E}_s(T)$, where T is the connected tree obtained from D by deleting some edges. Then by Corollary 3.2, $\mathcal{E}_s(T) \geq \mathcal{E}_s(S_n)$, and the equality holds if and only if $D \cong S_n$. □

Theorem 3.4. *Let D be a connected digraph in $\mathcal{O}_{n,m}$, $n-1 \leq m \leq \frac{3}{2}(n-1)$. If $D \ncong S_{n,m}$, then $\mathcal{E}_s(D) > \mathcal{E}_s(S_{n,m})$.*

Proof. We prove it by induction on m. If $m = n-1$, by Corollary3.2, the result holds. Suppose that the result holds for digraphs $D_0 \in \mathcal{O}_{n,m-1}$. We now consider $D \in \mathcal{O}_{n,m}$, $n \leq m \leq \frac{3}{2}(n-1)$.

Case 1. There are no pendant vertices in D. Then there must be a cycle $C \subseteq D$ which has only one vertex of degree more than 2. So there is an edge uv in C with $d(u) = d(v) = 2$. By Lemma 2.5,

$$a_{2k}(D) = a_{2k}(D-uv) + a_{2k-2}(D-u-v).$$

Since $m \geq n$, there exists a triangle $u'v'x$ on $S_{n,m}$ such that u' and v' have degree 2. Then

$$a_{2k}(S_{n,m}) = a_{2k}(S_{n,m-1}) + a_{2k-2}(S_{n-2,m-3}).$$

Clearly, $D - uv$, $D - u - v$ are connected, and $D - uv \in \mathcal{O}_{n,m-1}$, and $D - u - v \in \mathcal{O}_{n-2,m-3}$. By the induction hypothesis, $a_{2k}(D - uv) \geq a_{2k}(S_{n,m-1})$, $a_{2k-2}(D - u - v) \geq a_{2k-2}(S_{n-2,m-3})$. Thus we get that $a_{2k}(D) \geq a_{2k}(S_{n,m})$. Then $\mathcal{E}_s(D) \geq \mathcal{E}_s(S_{n,m})$, with equality if and only if $D \cong S_{n,m}$.

Case 2. There is a pendant edge uv in D with pendant vertex v. Then by Lemma 2.5,

$$a_{2k}(D) = a_{2k}(D - v) + a_{2k-2}(D - u - v).$$

If $S_{n,m}$ has no pendant edges, then m must be $\frac{3}{2}(n-1)$, but any digraph $D \in \mathcal{O}_{n,\frac{3}{2}(n-1)}$ has no pendant edges, a contradiction. So there must be a pendant edge $u'v'$ in $S_{n,m}$ with pendant vertex v'. Then

$$\begin{aligned} a_{2k}(S_{n,m}) &= a_{2k}(S_{n,m} - v') + a_{2k}(S_{n,m} - u' - v') \\ &= a_{2k}(S_{n-1,m-1}) + a_{2k-2}((m-n+1)P_2). \end{aligned}$$

First we consider the digraph $D - u - v$. Clearly, there are $m - n + 1$ cycles in D. For the x cycles which contain the vertex u with $1 \leq x \leq m - n + 1$, there are at least one edge left for each cycle in $D - u - v$, and the edges belonging to different cycles in D are now in different components. For the other $m - n + 1 - x$ cycles, there are at least three edges in each cycle. So $D - u - v$ contains $(m - n + 1)P_2$ as a subgraph. Then $a_{2k-2}(D - u - v) \geq a_{2k-2}((m - n + 1)P_2)$.

Since $D - v \in \mathcal{O}_{n-1,m-1}$, if $D - v$ contains no pendant vertex, then by the proof of Case 1, we have $a_{2k}(D - v) \geq a_{2k}(S_{n-1,m-1})$. Thus we get that $a_{2k}(D) \geq a_{2k}(S_{n,m})$. Then $\mathcal{E}_s(D) \geq \mathcal{E}_s(S_{n,m})$, with equality if and only if $D \cong S_{n,m}$. If $D - v$ contains a pendant vertex, then the problem is changed into comparing $a_{2k}(D - v)$ with $a_{2k}(S_{n-1,m-1})$. We repeat the above analysis until we get a digraph D' which contains no pendant vertex. Since $m \geq n$, the digraph D' exists. Then we know from the procedure that $a_{2k}(D) \geq a_{2k}(S_{n,m})$, that means $\mathcal{E}_s(D) \geq \mathcal{E}_s(S_{n,m})$.

The theorem is thus proved. $\square$

4. Maximal skew energy unicyclic digraphs with no even cycles

For undirected paths, Gutman and Polansky in [8] gave the following partial order relation:

Lemma 4.1. *Let $n = 4k,\ 4k+1,\ 4k+2,$ or $4k+3$. Then*

$$\begin{aligned} &P_n \succ P_2 \cup P_{n-2} \succ P_4 \cup P_{n-4} \succ \cdots \succ P_{2k} \cup P_{n-2k} \succ P_{2k+1} \cup P_{n-2k-1} \\ &\succ P_{2k-1} \cup P_{n-2k+1} \succ \cdots \succ P_3 \cup P_{n-3} \succ P_1 \cup P_{n-1}, \end{aligned}$$

where the graphs $G_1 \succ G_2$ means the energy of G_1 is more than or equal to that of G_2. By Lemma 3.1, the skew energy of digraphs have the same partial order relation, which is useful in our proof.

By the definition of $\mathcal{O}_{n,m}$, $\mathcal{O}_{n,n}$ is the class of connected digraphs with n vertices that contain an odd cycle C_ℓ as a subgraph, $3 \leq \ell \leq n$.

Theorem 4.2. *If n is odd, the digraph with maximal skew energy in $\mathcal{O}_{n,n}$ is C_n. If $n \equiv 0$ (mod 4), the digraph with maximal skew energy in $\mathcal{O}_{n,n}$ is $P_n^{\ell_0}$, $\ell_0 = n/2+1$. If $n \equiv 2$ (mod 4), the digraph with maximal skew energy in $\mathcal{O}_{n,n}$ is $P_n^{\ell_1}$, $\ell_1 = n/2$ or $n/2+2$.*

Proof. Let D be a digraph in $\mathcal{O}_{n,n}$ that contains the odd cycle C_ℓ. We first prove that $\mathcal{E}_s(D) \leq \mathcal{E}_s(P_n^\ell)$ by induction on n.

It is trivial that the result holds for $n-\ell = 0$ and $n-\ell = 1$. For $n-\ell = 2$, if $D \ncong P_n^\ell$, D must have a pendant edge uv with pendant vertex v. Clearly, $D - v \cong P_{\ell+1}^\ell$. By Lemma 2.5, $a_{2k}(D) = a_{2k}(D-v) + a_{2k-2}(D-u-v)$, $a_{2k}(P_n^\ell) = a_{2k}(P_{\ell+1}^\ell) + a_{2k-2}(C_\ell)$. Since $D-u-v$ is acyclic with ℓ vertices, $a_{2k-2}(D-u-v) = m(D-u-v,\ k-1) \leq m(P_\ell,\ k-1) < m(C_\ell, k-1) = a_{2k-2}(C_\ell)$. Thus the result holds for $n-\ell = 2$.

Let $p \geq 3$ and suppose that the result is true for $n-\ell < p$. Now we consider $n-\ell = p$. Since D is unicyclic but not a cycle, D must have a pendant edge uv with pendant vertex v. By Lemma 2.5,

$$\begin{aligned} a_{2k}(D) &= a_{2k}(D-v) + a_{2k-2}(D-u-v). \\ a_{2k}(P_n^\ell) &= a_{2k}(P_{n-1}^\ell) + a_{2k-2}(P_{n-2}^\ell) \end{aligned}$$

By the induction hypothesis, $a_{2k}(D-v) \leq a_{2k}(P_{n-1}^\ell)$. If $D-u-v$ contains the cycle C_ℓ, then by the induction hypothesis, we have $a_{2k-2}(D-u-v) \leq a_{2k-2}(P_{n-2}^\ell)$. If $D-u-v$ does not contain the cycle C_ℓ, then it is acyclic, $a_{2k-2}(D-u-v) = m(D-u-v,\ k-1) \leq m(P_{n-2},\ k-1) < m(P_{n-2}^\ell, k-1) = a_{2k-2}(P_{n-2}^\ell)$. Therefore, we get that $\mathcal{E}_s(D) \leq \mathcal{E}_s(P_n^\ell)$.

Now we prove that if n is odd, $\mathcal{E}_s(P_n^\ell) \leq \mathcal{E}_s(C_n)$. Let the vertex of degree 3 in C_ℓ be v, and one of its neighbors in C_ℓ be u. Choose any edge $u'v'$ in C_n. Then we have

$$\begin{aligned} a_{2k}(P_n^\ell) &= a_{2k}(P_n) + a_{2k-2}(P_{\ell-2} \cup P_{n-\ell}). \\ a_{2k}(C_n) &= a_{2k}(P_n) + a_{2k-2}(P_{n-2}). \end{aligned}$$

By Lemma 4.1, $a_{2k-2}(P_{\ell-2} \cup P_{n-\ell}) \leq a_{2k-2}(P_{n-2})$. Then $a_{2k}(P_n^\ell) \leq a_{2k}(C_n)$. Thus $\mathcal{E}_s(D) \leq \mathcal{E}_s(P_n^\ell) \leq \mathcal{E}_s(C_n)$.

If n is even, $C_n \notin \mathcal{O}_{n,n}$, and $\ell-2$, $n-\ell$ are both odd, then we compare $a_{2k}(P_n^\ell)$ for different ℓ. By Lemma 4.1, if $n \equiv 0$ $(mod\ 4)$, $3 \leq \ell \leq n$, $a_{2k-2}(P_{\ell-2} \cup P_{n-\ell})$ is maximal if and only if $\ell - 2 = n - \ell$, that is $\ell = \frac{n}{2}+1$. If $n \equiv 2$ $(mod\ 4)$, $3 \leq \ell \leq n$, $a_{2k-2}(P_{\ell-2} \cup P_{n-\ell})$ is maximal if and only if $\ell-2 = n-\ell \pm 2$, that is $\ell = \frac{n}{2}+2$ or $\frac{n}{2}$.

The proof is thus complete. □

5. Maximal skew energy bicyclic digraphs of even order with no even cycles

By the definition of $\mathcal{O}_{n,m}$, $\mathcal{O}_{n,n+1}$ is the class of connected digraphs with n vertices that contain exact two odd cycles C_ℓ, C_s as subgraphs, $3 \leq \ell, s \leq n$. We first compare the skew energy of a digraph D with that of $P_n^{\ell,s}$.

Lemma 5.1. *Let D be a digraph in $\mathcal{O}_{n,n+1}$ with exact two odd cycles C_ℓ, C_s, where n is even and $3 \leq \ell, s \leq n$. Then $\mathcal{E}_s(D) \leq \mathcal{E}_s(P_n^{\ell,s})$.*

Proof. We consider the following two cases.

Case 1. If C_ℓ and C_s have no common vertices, then C_ℓ and C_s are connected by a path P. We choose an edge uv on P satisfying that u is the vertex joining P with C_ℓ, and v is the neighbor of u on P, such that $D - uv$ contains two components that are unicyclic digraphs. Then we choose an edge $u'v'$ of $P_{n-\ell-s+2}$ on $P_n^{\ell,s}$ such that $P_n^{\ell,s} - u'v'$ contains two components with the same valencies of those of $D - uv$. By the proof of Theorem 4.2, we thus have

$$\begin{aligned} a_{2k}(D) &= a_{2k}(D - uv) + a_{2k-2}(D - u - v) \\ &\leq a_{2k}(P_n^{\ell,s} - u'v') + a_{2k-2}(P_n^{\ell,s} - u' - v') = a_{2k}(P_n^{\ell,s}). \end{aligned}$$

Then $\mathcal{E}_s(D) \leq \mathcal{E}_s(P_n^{\ell,s})$.

Case 2. If C_ℓ and C_s have a common vertex, since n is even and ℓ, s are odd, there is at least a tree planted on the cycles, without loss of generality, we suppose that at least one tree is planted on C_s.

Denote by $D - u$ the digraph obtained from D by deleting the vertex u together with all the edges incident with it. Then $D - u$ contains at least two components. Let the component containing $C_\ell - u$ be A_1, and the other components be A_2. Then we denote the digraph $D[A_1 \cup u]$ by B_1, and the digraph $D[A_2 \cup u]$ by B_2. If $v(B_2) = n_2$, then $n_2 \geq s + 1$. Let D' be the digraph obtained by joining the vertex u on B_1 with the leaf of $P^s_{n_2-1}$. Then we give an example of the underlying undirected graphs of the above digraphs.

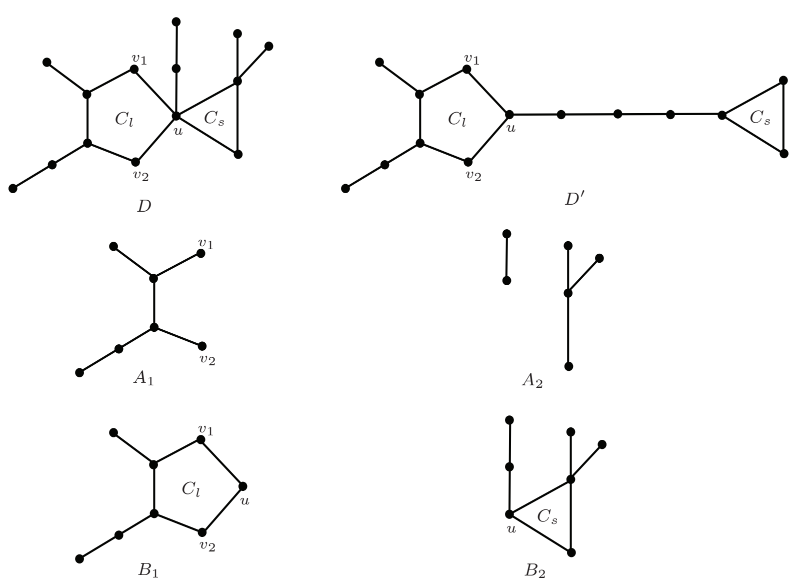

Figure 2. An example of the underlying undirected graphs of $D, D', A_1, A_2, B_1, B_2$.

Let the neighbors of u on C_ℓ be v_1 and v_2. Then by Lemma 2.5,

$$a_{2k}(D) = a_{2k}(D - uv_1) + a_{2k-2}(D - u - v_1),$$
$$a_{2k}(D') = a_{2k}(D' - uv_1) + a_{2k-2}(D' - u - v_1).$$

Clearly, $D - u - v_1 = (A_1 - v_1) \cup A_2$, and $D' - u - v_1 = (A_1 - v_1) \cup P^s_{n_2-1}$. Since A_2 is a forest with $n_2 - 1$ vertices, we have $a_{2k-2}(A_2) \le a_{2k-2}(P_{n_2-1}) < a_{2k-2}(P^s_{n_2-1})$, by Lemma 2.4, $a_{2k-2}(D-u-v_1) < a_{2k-2}(D' - u - v_1)$. Furthermore,

$$\begin{aligned} a_{2k}(D - uv_1) &= a_{2k}(D - uv_1 - uv_2) + a_{2k-2}(D - uv_1 - u - v_2), \\ &= a_{2k}(A_1 \cup B_2) + a_{2k-2}((A_1 - v_2) \cup A_2). \\ a_{2k}(D' - uv_1) &= a_{2k}(A_1 \cup P^s_{n_2}) + a_{2k-2}((A_1 - v_2) \cup P^s_{n_2-1}). \end{aligned}$$

Since B_2 is a unicyclic digraph with the cycle C_s, $a_{2k}(B_2) \le a_{2k}(P^s_{n_2})$. And $a_{2k-2}(A_2)$ $\le a_{2k-2}(P_{n_2-1}) < a_{2k-2}(P^s_{n_2-1})$. Then by Lemma 2.4, we have $a_{2k}(D - uv_1) < a_{2k}(D' - uv_1)$.

Thus we know that $a_{2k}(D) < a_{2k}(D')$, which means that $\mathcal{E}_s(D) < \mathcal{E}_s(D')$. Then by the proof of Case 1, we have $\mathcal{E}_s(D) < \mathcal{E}_s(D') \le \mathcal{E}_s(P^{\ell,s}_n)$.

The lemma is thus proved. □

Then we compare the skew energy of $P^{\ell,s}_n$ for different ℓ, s.

Lemma 5.2. *Let s, ℓ be odd integers with $s \ge \ell \ge 3$, where n is even and $n \ge s + \ell + 2$. Then $\mathcal{E}_s(P^{s,\ell}_n) < \mathcal{E}_s(P^{s,\ell+2}_n)$.*

Proof. By Lemma 2.5, we can easily get that

$$a_{2k}(P^{s,\ell}_n) = a_{2k}(P^s_n) + a_{2k-2}(P_{\ell-2} \cup P_{n-\ell}) + a_{2k-4}(P_{\ell-2} \cup P_{s-2} \cup P_{n-s-\ell}),$$
$$a_{2k}(P^{s,\ell+2}_n) = a_{2k}(P^s_n) + a_{2k-2}(P_\ell \cup P_{n-\ell-2}) + a_{2k-4}(P_\ell \cup P_{s-2} \cup P_{n-s-\ell-2}).$$

Since n is even, s, ℓ are odd, we have $\ell - 2,\ s - 2,\ n - \ell,\ n - \ell - 2$ are odd and $n - s - \ell,\ n - s - \ell - 2$ are even. From Lemma 4.1, $a_{2k-2}(P_{\ell-2} \cup P_{n-\ell}) < a_{2k-2}(P_\ell \cup P_{n-\ell-2})$, for $n - \ell - 2 \ge s \ge \ell > \ell - 2$. And $\ell - 2 < \ell$, $n - s - \ell > n - s - \ell - 2$. Then $a_{2k-4}(P_{\ell-2} \cup P_{s-2} \cup P_{n-s-\ell}) < a_{2k-4}(P_\ell \cup P_{s-2} \cup P_{n-s-\ell-2})$. Therefore, $a_{2k}(P^{s,\ell}_n) < a_{2k}(P^{s,\ell+2}_n)$. Then we have $\mathcal{E}_s(P^{s,\ell}_n) < \mathcal{E}_s(P^{s,\ell+2}_n)$. □

For convenience, we introduce the following notations, which will be used in our next proof.

$$\begin{aligned}
&Y_1 = \frac{1+\sqrt{1+4x^2}}{2}, \qquad Y_2 = \frac{1-\sqrt{1+4x^2}}{2},\\
&A_1 = \frac{x^2+1-Y_2}{Y_1^2+x^2}, \qquad A_2 = \frac{x^2+1-Y_1}{Y_2^2+x^2},\\
&B_1 = A_1 + x^2A_1^2Y_1^{-2} - x^{2\ell-2}A_1A_2Y_1^{-2\ell+2},\\
&B_2 = A_2 + x^2A_2^2Y_2^{-2} - x^{2\ell-2}A_1A_2Y_2^{-2\ell+2},\\
&C_1 = A_1 + 2x^2A_1^2Y_1^{-2} + x^4A_1^3Y_1^{-4} - x^{2s-2}A_1A_2Y_1^{-2s+2} - x^{2\ell-2}A_1A_2Y_1^{-2\ell+2}\\
&\qquad -x^{2s}A_1^2A_2Y_1^{-2s} - x^{2\ell}A_1^2A_2Y_1^{-2\ell} + x^{2s+2\ell-4}A_1A_2^2Y_1^{-2s-2\ell+4},\\
&C_2 = A_2 + 2x^2A_2^2Y_2^{-2} + x^4A_2^3Y_2^{-4} - x^{2s-2}A_1A_2Y_2^{-2s+2} - x^{2\ell-2}A_1A_2Y_2^{-2\ell+2}\\
&\qquad -x^{2s}A_1A_2^2Y_2^{-2s} - x^{2\ell}A_1A_2^2Y_2^{-2\ell} + x^{2s+2\ell-4}A_1^2A_2Y_2^{-2s-2\ell+4}.
\end{aligned}$$

It is easy to verify that $Y_1+Y_2=1$, $Y_1Y_2=-x^2$, $A_1A_2=\frac{x^2}{1+4x^2}$.

Lemma 5.3. *For $s,\ell\geq 3$, $n\geq s+\ell$, the signless matching polynomial of P_n, P_n^{ℓ} and $P_n^{s,\ell}$ have the following forms:*

$$\begin{aligned}
m^+(P_n,x) &= A_1(x)(Y_1(x))^n + A_2(x)(Y_2(x))^n,\\
m^+(P_n^{\ell},x) &= B_1(x)(Y_1(x))^n + B_2(x)(Y_2(x))^n,\\
m^+(P_n^{s,\ell},x) &= C_1(x)(Y_1(x))^n + C_2(x)(Y_2(x))^n.
\end{aligned}$$

Proof. By Lemma 2.9, we know that $m^+(P_n,x)$ satisfies the recursive formula $f(n,x)=f(n-1,x)+x^2f(n-2,x)$. Therefore, the form of the general solution of the linear homogeneous recursive relation is $f(n,x)=F_1(x)(Y_1(x))^n+F_2(x)(Y_2(x))^n$. By some elementary calculations, together with the initial values

$$m^+(P_2,x)=1+x^2, \quad m^+(P_3,x)=1+2x^2,$$

we can easily obtain that $F_i(x)=A_i(x)$, $i=1,2$. From Lemmas 2.7 and 2.8, we deduce that

$$\begin{aligned}
m^+(P_n^{\ell},x) &= m^+(P_n,x) + x^2m^+(P_{\ell-2},x)m^+(P_{n-\ell},x),\\
m^+(P_n^{s,\ell},x) &= m^+(P_n^{\ell},x) + x^2m^+(P_{s-2},x)m^+(P_{n-s}^{\ell},x).
\end{aligned}$$

Then by means of some elementary calculations, we can get the above formulas for $m^+(P_n^{\ell},x)$ and $m^+(P_n^{s,\ell},x)$. □

Before giving the following results, we state some knowledge on real analysis, for which we refer to [17].

Lemma 5.4. *For any real number $X>-1$, we have*

$$\frac{X}{1+X}\leq \log(1+X)\leq X.$$

Lemma 5.5. *Let s,ℓ be odd integers with $s\geq\ell\geq 3$, $s\geq \ell+4$, where n is even and $n\geq s+\ell$. Then $\mathcal{E}_s(P_n^{s,\ell})<\mathcal{E}_s(P_n^{s-2,\ell+2})$.*

Proof. From Eq. (2.2), we get that

$$\begin{aligned}&\mathcal{E}_s(P_n^{s,\ell})-\mathcal{E}_s(P_n^{s-2,\ell+2})\\ =\ &\frac{2}{\pi}\int_0^{+\infty}\frac{1}{x^2}\log\frac{m^+(P_n^{s,\ell},x)}{m^+(P_n^{s-2,\ell+2},x)}dx\\ =\ &\frac{2}{\pi}\int_0^{+\infty}\frac{1}{x^2}\log\left(1+\frac{m^+(P_n^{s,\ell},x)-m^+(P_n^{s-2,\ell+2},x)}{m^+(P_n^{s-2,\ell+2},x)}\right)dx.\end{aligned}$$

Since $m^+(P_n^{s,\ell},x)>0$ and $m^+(P_n^{s-2,\ell+2},x)>0$ for all x, we have

$$\frac{m^+(P_n^{s,\ell},x)-m^+(P_n^{s-2,\ell+2},x)}{m^+(P_n^{s-2,\ell+2},x)}=\frac{m^+(P_n^{s,\ell},x)}{m^+(P_n^{s-2,\ell+2},x)}-1>-1.$$

Therefore, by Lemma 5.4

$$\log\left(1+\frac{m^+(P_n^{s,\ell},x)-m^+(P_n^{s-2,\ell+2},x)}{m^+(P_n^{s-2,\ell+2},x)}\right)\le\frac{m^+(P_n^{s,\ell},x)-m^+(P_n^{s-2,\ell+2},x)}{m^+(P_n^{s-2,\ell+2},x)}.$$

We assume $m^+(P_n^{s-2,\ell+2},x)=C_1'(x)(Y_1(x))^n+C_2'(x)(Y_2(x))^n$. Then

$$\begin{aligned}C_1'&=A_1+2x^2A_1^2Y_1^{-2}+x^4A_1^3Y_1^{-4}-x^{2s-6}A_1A_2Y_1^{-2s+6}-x^{2\ell+2}A_1A_2Y_1^{-2\ell-2}\\&\quad-x^{2s-4}A_1^2A_2Y_1^{-2s+4}-x^{2\ell+4}A_1^2A_2Y_1^{-2\ell-4}+x^{2s+2\ell-4}A_1A_2^2Y_1^{-2s-2\ell+4},\\ C_2'&=A_2+2x^2A_2^2Y_2^{-2}+x^4A_2^3Y_2^{-4}-x^{2s-6}A_1A_2Y_2^{-2s+6}-x^{2\ell+2}A_1A_2Y_2^{-2\ell-2}\\&\quad-x^{2s-4}A_1A_2^2Y_2^{-2s+4}-x^{2\ell+4}A_1A_2^2Y_2^{-2\ell-4}+x^{2s+2\ell-4}A_1^2A_2Y_2^{-2s-2\ell+4}.\end{aligned}$$

Thus we get that

$$\begin{aligned}&\Delta C_1=C_1-C_1'\\ =\ &-x^{2s-2}A_1A_2Y_1^{-2s+2}-x^{2\ell-2}A_1A_2Y_1^{-2\ell+2}-x^{2s}A_1^2A_2Y_1^{-2s}+x^{2s-6}A_1A_2Y_1^{-2s+6}\\&-x^{2\ell}A_1^2A_2Y_1^{-2\ell}+x^{2\ell+2}A_1A_2Y_1^{-2\ell-2}+x^{2s-4}A_1^2A_2Y_1^{-2s+4}+x^{2\ell+4}A_1^2A_2Y_1^{-2\ell-4}\\ =\ &(Y_1^4-x^4)(Y_1^{2\ell+4-2s}-x^{2\ell+4-2s})(x^{2s-6}A_1A_2Y_1^{-2\ell-2}+x^{2s-4}A_1^2A_2Y_1^{-2\ell-4}).\end{aligned}$$

By our definition, we know that $Y_1=\frac{1+\sqrt{1+4x^2}}{2}>|x|\ge 0$, $2\ell+4-2s<0$. Therefore $Y_1^4-x^4>0$, $Y_1^{2\ell+4-2s}-x^{2\ell+4-2s}<0$. And $A_1=\frac{x^2+1-Y_2}{Y_1^2+x^2}=\frac{2x^2+1+\sqrt{1+4x^2}}{2(Y_1^2+x^2)}>0$, $A_1A_2=\frac{x^2}{1+4x^2}>0$, then $x^{2s-6}A_1A_2Y_1^{-2\ell-2}+x^{2s-4}A_1^2A_2Y_1^{-2\ell-4}>0$ for all x. From the above analysis, we finally get that $\Delta C_1<0$.

By a similar method, we can get that $\Delta C_2=C_2-C_2'<0$. Thus for any x and all even n,

$$m^+(P_n^{s,\ell},x)-m^+(P_n^{s-2,\ell+2},x)=\Delta C_1Y_1^n+\Delta C_2Y_2^n<0.$$

Then

$$\log\left(1+\frac{m^+(P_n^{s,\ell},x)-m^+(P_n^{s-2,\ell+2},x)}{m^+(P_n^{s-2,\ell+2},x)}\right)\le\frac{m^+(P_n^{s,\ell},x)-m^+(P_n^{s-2,\ell+2},x)}{m^+(P_n^{s-2,\ell+2},x)}<0.$$

Therefore,

$$\begin{aligned}&\mathcal{E}_s(P_n^{s,\ell})-\mathcal{E}_s(P_n^{s-2,\ell+2})\\ = \quad &\frac{2}{\pi}\int_0^{+\infty}\frac{1}{x^2}\log\left(1+\frac{m^+(P_n^{s,\ell},x)-m^+(P_n^{s-2,\ell+2},x)}{m^+(P_n^{s-2,\ell+2},x)}\right)dx<0.\end{aligned}$$

The lemma is thus proved. □

So for any digraph D in $\mathcal{O}_{n,n+1}$ with exact two odd cycles C_ℓ, C_s, $3\le \ell, s\le n$, n even, by Lemma 5.1, $\mathcal{E}_s(D)\le \mathcal{E}_s(P_n^{\ell,s})$. Then by using Lemma 5.2 repeatedly, $\mathcal{E}_s(P_n^{s,\ell})<\mathcal{E}_s(P_n^{s',\ell'})$, where s',ℓ' are odd, $s'\ge s,\ \ell'\ge \ell,\ s'+\ell'=n$. Finally, we use Lemma 5.5 repeatedly, and then deduce the following result.

Theorem 5.6. *let n be an even integer, if $n\equiv 0\ (mod\ 4)$, the digraphs with maximal skew energy in $\mathcal{O}_{n,n+1}$ is $P_n^{\ell,\ell-2}$, $\ell=n/2+1$. If $n\equiv 2\ (mod\ 4)$, the digraphs with maximal skew energy in $\mathcal{O}_{n,n+1}$ is $P_n^{\ell',\ell'}$, $\ell'=n/2$.*

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