

## ON ORIENTED GRAPHS WITH MINIMAL SKEW ENERGY\*

SHICAI GONG<sup>†</sup>, XUELIANG LI<sup>‡</sup>, AND GUANGHUI XU<sup>§</sup>

**Abstract.** Let  $S(G^{\sigma})$  be the skew-adjacency matrix of an oriented graph  $G^{\sigma}$ . The skew energy of  $G^{\sigma}$  is the sum of all singular values of its skew-adjacency matrix  $S(G^{\sigma})$ . This paper first establishes an integral formula for the skew energy of an oriented graph. Then, it determines all oriented graphs with minimal skew energy among all connected oriented graphs on n vertices with  $m (n \leq m < 2(n-2))$  arcs, which is analogous to the conjecture for the energy of undirected graphs proposed by Caporossi et al. [G. Caporossi, D. Cvetković, I. Gutman, and P. Hansen. Variable neighborhood search for extremal graphs. 2. Finding graphs with external energy. J. Chem. Inf. Comput. Sci., 39:984–996, 1999.].

Key words. Oriented graph, Graph energy, Skew energy, Skew-adjacency matrix, Skew characteristic polynomial.

AMS subject classifications. 05C50, 15A18.

**1. Introduction.** Let  $G^{\sigma}$  be a digraph that arises from a simple undirected graph G with an orientation  $\sigma$ , which assigns to each edge of G a direction so that  $G^{\sigma}$  becomes an oriented graph, or a directed graph. The undirected graph G is called the underlying graph of  $G^{\sigma}$ . Let  $G^{\sigma}$  be an undirected graph with vertex set  $V(G^{\sigma}) = \{v_1, v_2, \ldots, v_n\}$ . Denote by (u, v) an arc, of  $G^{\sigma}$ , with tail u and head v. The skew-adjacency matrix related to  $G^{\sigma}$  is the  $n \times n$  matrix  $S(G^{\sigma}) = [s_{ij}]$ , where the (i, j) entry satisfies:

$$s_{ij} = \begin{cases} 1, & \text{if } (\mathbf{v}_i, \mathbf{v}_j) \in \mathbf{G}^{\sigma} ;\\ -1, & \text{if } (\mathbf{v}_j, \mathbf{v}_i) \in \mathbf{G}^{\sigma} ;\\ 0, & \text{otherwise.} \end{cases}$$

The skew energy of an oriented graph  $G^{\sigma}$ , introduced by Adiga, Balakrishnan and So in [1] and denoted by  $\mathcal{E}_S(G^{\sigma})$ , is the sum of all singular values of  $S(G^{\sigma})$ . Because the skew-adjacency matrix  $S(G^{\sigma})$  is skew-symmetric, the eigenvalues  $\{\lambda_1, \lambda_2, \ldots, \lambda_n\}$  of

<sup>\*</sup>Received by the editors on April 20, 2013. Accepted for publication on August 10, 2014. Handling Editor: Bryan L. Shader.

<sup>&</sup>lt;sup>†</sup>School of Science, Zhejiang A&F University, Hangzhou, 311300, P.R. China (scgong@zafu.edu.cn). Supported by Zhejiang Provincial Natural Science Foundation of China (LY12A01016) and Natural Science Foundation of China (no. 11301484).

<sup>&</sup>lt;sup>‡</sup>Center for Combinatorics and LPMC-TJKLC, Nankai University, Tianjin 300071, P.R. China (lxl@nankai.edu.cn). Supported by National Natural Science Foundation of China (no. 10831001).

<sup>&</sup>lt;sup>§</sup>School of Science, Zhejiang A&F University, Hangzhou, 311300, P.R. China (ghxu@zafu.edu.cn). Supported by National Natural Science Foundation of China (no. 11171373).

S.C. Gong, X.L. Li, and G.H. Xu

 $S(G^{\sigma})$  are all purely imaginary numbers. Consequently, the skew energy  $\mathcal{E}_S(G^{\sigma})$  is the sum of the modulus of its eigenvalues, i.e.,

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

which has the same expression as that of the energy of an undirected graph with respect to its adjacency matrix; see e.g. [14].

The work on the energy of a graph can be traced back to 1970's [10] when Gutman investigated the energy with respect to the adjacency matrix of an undirected graph, which has a still older chemical origin; see e.g. [6]. Much attention has been devoted to the energy of the adjacency matrix of a graph; see e.g. [2, 3, 4, 7, 12, 13, 11, 18, 21, 22, 25], and the references cited therein. For undirected graphs, Caporossi, Cvetković, Gutman and Hansen [5] propose the following conjecture.

CONJECTURE 1. Let G be the graph with minimum energy among all connected graphs with  $n \ge 6$  vertices and m  $(n-1 \le m \le 2(n-2))$  edges. Then G is  $O_{n,m}$ if  $m \le n + \lfloor \frac{n-7}{2} \rfloor$ , and  $B_{n,m}$  otherwise, where  $O_{n,m}$  and  $B_{n,m}$  are respectively the underlying graphs of the oriented graphs  $O_{n,m}^+$  and  $B_{n,m}^+$  given in Fig. 1.1.

This conjecture was proved to be true for m = n - 1 and m = 2(n - 2) by Caporossi et al. [5, Theorem 1], and m = n by Hou [17]. In [22], Li, Zhang and Wang confirmed this conjecture for bipartite graphs. Conjecture 1 has not yet been solved completely.

Recently, other versions of graph energy were introduced in the mathematical literature, such as Laplacian energy [16], signless Laplacian energy [15] and skew energy [1].

In [1], Adiga et al. obtained the skew energies of directed cycles under different orientations and showed that the skew energy of a directed tree is independent of its orientation, which is equal to the energy of its underlying tree. Naturally, the following question is interesting:

QUESTION: Denote by M a class of oriented graphs. Which oriented graphs have the extremely skew energy among all oriented graphs of M?

Hou et al. [20] determined the oriented unicyclic graphs with the maximal and minimal skew energies. Zhu [26] determined the oriented unicyclic graphs with the first  $\lfloor \frac{n-9}{2} \rfloor$  largest skew energies. Shen et al. [23] determined the bicyclic graphs with the maximal and minimal energies. Gong and Xu [9] determined the 3-regular graphs with the optimum skew energy, and Tian [24] determined the hypercubes with the optimum skew energy. In the following, we will study the minimal skew energy graphs of order n and size m.

694

ELA

#### On Oriented Graphs With Minimal Skew Energy

First we need some notation. Denote by  $K_n$ ,  $S_n$  and  $C_n$  the complete undirected graph, the undirected star and the undirected cycle on n vertices, respectively. Let  $O_{n,m}^+$  be the oriented graph on n vertices that is obtained from the oriented star  $S_n^{\sigma}$ by inserting m - n + 1 arcs between an arbitrary pendent vertex and other m - n + 1pendent vertices; see Fig. 1.1, where  $n - 1 \leq m \leq 2n - 4$ ,  $v_1$  is the tail of each arc incident to it and  $v_2$  is the head of each arc incident to it, and  $B_{n,m}^+$ , the oriented graph obtained from  $O_{n,m+1}^+$  by deleting the arc  $(v_1, v_2)$ . Denote by  $O_{n,m}$  and  $B_{n,m}$ the underlying graphs of  $O_{n,m}^+$  and  $B_{n,m}^+$ , respectively. Notice that both  $O_{n,m}^+$  and  $B_{n,m}^+$  contain n vertices and m arcs.



Fig. 1.1. Oriented graphs  $O_{n,m}^+$  and  $B_{n,m}^+$ .

In this paper, we first establish an integral formula for the skew energy of an oriented graph. Then, we study the question above and determine all oriented graphs with minimal skew energy among all connected oriented digraphs on n vertices with m ( $n \le m < 2(n-2)$ ) arcs. Interestingly, our result is an analogy of Conjecture 1.

THEOREM 1.1. Let  $G^{\sigma}$  be an oriented graph with minimal skew energy among all oriented graphs with n vertices and m  $(n \leq m < 2(n-2))$  arcs. Then, up to isomorphism,  $G^{\sigma}$  is

- (1)  $O_{n,m}^+$  if  $m < \frac{3n-5}{2}$ ;
- (2) either  $B_{n,m}^+$  or  $O_{n,m}^+$  if  $m = \frac{3n-5}{2}$ ;
- (3)  $B_{n,m}^+$  otherwise.

2. Integral formula for the skew energy. In this section, based on the formula established by Adiga et al. [1], we derive an integral formula for the skew energy of an oriented graph, the formula is an analogy of the Coulson integral formula for the energy of an undirected graph. First we introduce some notation and preliminary results.

An even cycle C in an oriented graph  $G^{\sigma}$  is oddly oriented if for either choice of

695

### S.C. Gong, X.L. Li, and G.H. Xu

direction of traversal around C, the number of edges of C directed in the direction of the traversal is odd. Since C is even, this is clearly independent of the initial choice of direction of traversal. Otherwise, such an even cycle C is called as *evenly oriented*. (Here we do not involve the parity of the cycle with length odd. The reason is that it depends on the initial choice of direction of traversal.)

A "basic oriented graph" is an oriented graph whose components are even cycles and/or complete oriented graphs with exactly two vertices.

Denote by  $\phi(G^{\sigma}, x)$  the *skew characteristic polynomial* of an oriented graph  $G^{\sigma}$ , which is defined as

$$\phi(G^{\sigma}, x) = \det(xI_n - S(G^{\sigma})) = \sum_{i=0}^n (-1)^i a_i(G^{\sigma}) x^{n-i},$$

where  $I_n$  denotes the identity matrix of order n. The following result is a cornerstone of our discussion below, which determines all coefficients of the skew characteristic polynomial of an oriented graph in terms of its basic oriented subgraphs; see [19, Theorem 2.4] for an independent version.

LEMMA 2.1. [8, Corollary 2.3] Let  $G^{\sigma}$  be an oriented graph on *n* vertices, and let the skew characteristic polynomial of  $G^{\sigma}$  be

$$\phi(G^{\sigma},\lambda) = \sum_{i=0}^{n} (-1)^{i} a_{i} \lambda^{n-i} = \lambda^{n} - a_{1} \lambda^{n-1} + a_{2} \lambda^{n-2} + \dots + (-1)^{n-1} a_{n-1} \lambda + (-1)^{n} a_{n}.$$

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

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

where the summation is over all basic oriented subgraphs  $\mathscr{H}$  of  $G^{\sigma}$  having *i* vertices and  $c^+$  and *c* are respectively the number of evenly oriented even cycles and even cycles contained in  $\mathscr{H}$ .

Let G = (V(G), E(G)) be a graph, directed or not, on *n* vertices. Then denote by  $\Delta(G)$  the maximum degree of *G* and set  $\Delta(G^{\sigma}) = \Delta(G)$ . An *r*-matching in a graph *G* is a subset of *r* edges such that every vertex of V(G) is incident to at most one edge in it. Denote by M(G, r) the number of all *r*-matchings in *G* and set M(G, 0) = 1.

Denote by q(G) the number of quadrangles in a undirected graph G. As a consequence of Lemma 2.1, we have

THEOREM 2.2. Let  $G^{\sigma}$  be an oriented graph containing n vertices and m arcs. Suppose

$$\phi(G^{\sigma},\lambda) = \sum_{i=0}^{n} (-1)^{i} a_{i}(G^{\sigma})\lambda^{n-i}.$$

696



On Oriented Graphs With Minimal Skew Energy

Then  $a_0(G^{\sigma}) = 1$ ,  $a_2(G^{\sigma}) = m$  and  $a_4(G^{\sigma}) \ge M(G,2) - 2q(G)$ , with equality if and only if all oriented quadrangles of  $G^{\sigma}$  are evenly oriented.

*Proof.* The result follows from Lemma 2.1 and the fact that each arc corresponds a basic oriented graph having 2 vertices, and each basic oriented graph having 4 vertices is either a 2-matching or a quadrangle.  $\Box$ 

Furthermore, as well-known, the eigenvalues of an arbitrary real skew symmetric matrix are all purely imaginary numbers and occur in conjugate pairs. Henceforth, Lemma 2.1 can be strengthened as follows, which will provide much convenience for our discussion below.

LEMMA 2.3. Let  $G^{\sigma}$  be an oriented graph of order n. Then each coefficient of the skew characteristic polynomial

$$\phi(G^{\sigma},\lambda) = \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} a_{2i}(G^{\sigma})\lambda^{n-2i}$$

satisfies  $a_{2i}(G^{\sigma}) \ge 0$  for each  $i(0 \le i \le \lfloor \frac{n}{2} \rfloor)$ .

*Proof.* By pairing eigenvalues of  $G^{\sigma}$  in conjugate pairs we see that the characteristic polynomial of  $G^{\sigma}$  has the form  $x^k(x^2 + a_1^2) \cdots (x^2 + a_r^2)$  for some k, r and  $a_i$ 's. It now follows that  $a_{2i+1} = 0$  for each i, and  $a_{2i} \ge 0$  for each i.  $\Box$ 

For an oriented graph  $G^{\sigma}$  on n vertices, an integral formula for the skew energy in terms of the skew characteristic polynomial  $\phi(G^{\sigma}, \lambda)$  and its derivative is given by [1],

$$\mathscr{E}_{s}(G^{\sigma}) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \left[ n + \lambda \frac{\phi'(G^{\sigma}, -\lambda)}{\phi(G^{\sigma}, -\lambda)} \right] d\lambda.$$
(2.1)

However, using the above integral, it is by no means easy to calculate the skew energy of an oriented graph. Hence, it is rather important to establish some other more simpler formula.

Applying to (2.1) the fact that the coefficient  $a_i = 0$  for each odd *i* from Lemma 2.1 and replacing  $\lambda$  by  $-\lambda$ , we have

$$\mathscr{E}_s(G^{\sigma}) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \left[ n - \lambda \frac{\phi'(G^{\sigma}, \lambda)}{\phi(G^{\sigma}, \lambda)} \right] d\lambda.$$

Meanwhile, note that

$$\frac{\phi'(G^{\sigma},\lambda)}{\phi(G^{\sigma},\lambda)}d\lambda = d\ln\phi(G^{\sigma},\lambda).$$

ELA

S.C. Gong, X.L. Li, and G.H. Xu

Then

$$\mathscr{E}_{s}(G^{\sigma}) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \left[ n - \lambda \frac{\phi'(G^{\sigma}, \lambda)}{\phi(G^{\sigma}, \lambda)} \right] d\lambda$$
  
=  $\frac{1}{\pi} \int_{-\infty}^{+\infty} \left[ n - \lambda (\frac{d}{d\lambda}) \ln \phi(G^{\sigma}, \lambda) \right] d\lambda.$ 

Therefore, we have the following result.

THEOREM 2.4. Let  $G^{\sigma}$  be an oriented graph with order n. Then

$$\mathscr{E}_{s}(G^{\sigma}) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \lambda^{-2} \ln \psi(G^{\sigma}, \lambda) d\lambda, \qquad (2.2)$$

where

$$\psi(G^{\sigma},\lambda) = \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} a_{2i}(G^{\sigma})\lambda^{2i}$$

and  $a_{2i}(G^{\sigma})$  denotes the coefficient of  $\lambda^{n-2i}$  in the skew characteristic polynomial  $\phi(G^{\sigma}, \lambda)$ .

*Proof.* Let both  $G_1^{\sigma_1}$  and  $G_2^{\sigma_2}$  be oriented graphs with order *n*. ( $G_1$  perhaps equals  $G_2$ .) Applying (2.2), we have

$$\mathscr{E}_s(G_1^{\sigma_1}) - \mathscr{E}_s(G_2^{\sigma_2}) = -\frac{1}{\pi} \int_{-\infty}^{+\infty} \lambda(\frac{d}{d\lambda}) \ln\left[\frac{\phi(G_1^{\sigma_1}, \lambda)}{\phi(G_2^{\sigma_2}, \lambda)}\right] d\lambda.$$

Using partial integration, we have

$$\mathscr{E}_{s}(G_{1}^{\sigma_{1}}) - \mathscr{E}_{s}(G_{2}^{\sigma_{2}}) = -\frac{\lambda}{\pi} \ln\left[\frac{\phi(G_{1}^{\sigma_{1}},\lambda)}{\phi(G_{2}^{\sigma_{2}},\lambda)}\right]\Big|_{-\infty}^{+\infty} + \frac{1}{\pi} \int_{-\infty}^{+\infty} \ln\left[\frac{\phi(G_{1}^{\sigma_{1}},\lambda)}{\phi(G_{2}^{\sigma_{2}},\lambda)}\right] d\lambda.$$

Notice that

$$\frac{\lambda}{\pi} \ln \left[ \frac{\phi(G_1^{\sigma_1}, \lambda)}{\phi(G_2^{\sigma_2}, \lambda)} \right] |_{-\infty}^{+\infty} = 0.$$

Hence,

$$\mathscr{E}_s(G_1^{\sigma_1}) - \mathscr{E}_s(G_2^{\sigma_2}) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \ln\left[\frac{\phi(G_1^{\sigma_1}, \lambda)}{\phi(G_2^{\sigma_2}, \lambda)}\right] d\lambda.$$

Suppose now that  $G_2^{\sigma_2}$  is the null oriented graph; that is,  $G_2^{\sigma_2}$  is an oriented graph containing *n* isolated vertices. Then  $\phi(G_2^{\sigma_2}, \lambda) = \lambda^n$ , and thus,  $\mathscr{E}_s(G_2^{\sigma_2}) = 0$ . After an appropriate change of variables we can derive

$$\mathscr{E}_s(G_1^{\sigma_1}) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \lambda^{-2} \ln \psi(G_1^{\sigma_1}, \lambda) d\lambda.$$

The result now follows.  $\square$ 

### On Oriented Graphs With Minimal Skew Energy

**3.** The proof of Theorem 1.1. From Theorem 2.4, for an oriented graph  $G^{\sigma}$  on *n* vertices, the skew energy  $\mathcal{E}_s(G^{\sigma})$  is a strictly monotonically increasing function of the coefficients  $a_{2k}(G^{\sigma})(k = 0, 1, \ldots, \lfloor \frac{n}{2} \rfloor)$ , since for each *i* the coefficient of  $\lambda^{n-i}$  in the characteristic polynomial  $\phi(G^{\sigma}, \lambda)$ , as well as  $\psi(G^{\sigma}, \lambda)$ , satisfies  $a_i(G^{\sigma}) \geq 0$  by Lemma 2.3. Thus, similar to comparing two undirected graphs with respect to their energies, we define the quasi-ordering relation " $\preceq$ " of two oriented graphs with respect to their skew energies as follows.

Let  $G_1^{\sigma_1}$  and  $G_2^{\sigma_2}$  be oriented graphs of order n.  $(G_1$  is not necessarily different from  $G_2$ .) If  $a_{2i}(G_1^{\sigma_1}) \leq a_{2i}(G_2^{\sigma_2})$  for all i with  $0 \leq i \leq \lfloor \frac{n}{2} \rfloor$ , then we write that  $G_1^{\sigma_1} \leq G_2^{\sigma_2}$ .

Furthermore, if  $G_1^{\sigma_1} \preceq G_2^{\sigma_2}$  and there exists at least one index *i* such that  $a_{2i}(G_1^{\sigma_1}) < a_{2i}(G_2^{\sigma_2})$ , then we write that  $G_1^{\sigma_1} \prec G_2^{\sigma_2}$ . If  $a_{2i}(G_1^{\sigma_1}) = a_{2i}(G_2^{\sigma_2})$  for all *i*, we write  $G_1^{\sigma_1} \sim G_2^{\sigma_2}$ . Note that there are non-isomorphic oriented graphs  $G_1^{\sigma_1}$  and  $G_2^{\sigma_2}$  such that  $G_1^{\sigma_1} \sim G_2^{\sigma_2}$ , which implies that " $\preceq$ " is not a partial ordering.

According to the integral formula (2.2), we have, for two oriented graphs  $G_1^{\sigma_1}$  and  $G_2^{\sigma_2}$  of order n, that

$$G_1^{\sigma_1} \preceq G_2^{\sigma_2} \Longrightarrow \mathcal{E}_s(G_1^{\sigma_1}) \le \mathcal{E}_s(G_2^{\sigma_2})$$

and

698

$$G_1^{\sigma_1} \prec G_2^{\sigma_2} \Longrightarrow \mathcal{E}_s(G_1^{\sigma_1}) < \mathcal{E}_s(G_2^{\sigma_2}).$$
(3.1)

In the following, by discussing the relation " $\succeq$ ", we compare the skew energies for two oriented graphs and then complete the proof of Theorem 1.1.

First, by a direct calculation we have

$$\phi(O_{n,m}^{+}) = \lambda^{n} + m\lambda^{n-2} + (m-n+1)(2n-m-3)\lambda^{n-4}, \qquad (3.2)$$

and

$$\phi(B_{n,m}^+) = \lambda^n + m\lambda^{n-2} + (m-n+2)(2n-m-4)\lambda^{n-4}.$$
(3.3)

Denote by  $G^{\sigma}(n,m)$  and G(n,m) the sets of all connected oriented graphs and undirected graphs with *n* vertices and *m* edges, respectively. The following results on undirected graphs are needed.

LEMMA 3.1. Let  $n \ge 5$  and  $G \in G(n,m)$  be an arbitrary connected undirected graph containing n vertices and m edges with  $n \le m < 2(n-2)$ . Then  $q(G) \le \binom{m-n+2}{2}$ , where q(G) denotes the number of quadrangles contained in G.

S.C. Gong, X.L. Li, and G.H. Xu

*Proof.* We prove this result by induction on m.

The result is obvious for m = n. So we suppose that n < m < 2(n-2) and the result is true for smaller m.

Let e be an edge of G and  $q_G(e)$  denote the number of quadrangles containing the edge e. Suppose e = (u, v). Let U be the set of neighbors of u except v, and Vthe set of neighbors of v except u. Then there are just  $q_G(e)$  edges between U and V. Let X be the subset of U such that each vertex in X is incident to some of the above  $q_G(e)$  edges and Y be the subset of V defined similarly to X. Assume |X| = x and |Y| = y. Let  $G_0$  be the subgraph of G induced by  $V(G_0) = u \cup v \cup X \cup Y$ . Then there are at least  $q_G(e) + x + y + 1$  edges and exactly x + y + 2 vertices in  $G_0$ . In order for the remaining vertices to connect to  $G_0$ , the number of remaining edges must be not less than that of the remaining vertices. Thus,

$$m - (q_G(e) + x + y + 1) \ge n - (x + y + 2),$$

or equivalently,

$$q_G(e) \le m - n + 1$$

By the induction hypothesis,

$$q(G-e) \le \begin{pmatrix} (m-1)-n+2\\ 2 \end{pmatrix} = \begin{pmatrix} m-n+1\\ 2 \end{pmatrix}.$$

Thus, we have

$$q(G) = q_G(e) + q(G-e) \le m - n + 1 + \binom{m - n + 1}{2} = \binom{m - n + 2}{2}.$$

Hence, the result follows.  $\square$ 

By a similar method, we can show the following.

LEMMA 3.2. Let  $n \ge 5$  and  $G \in G(n,m)$  be an arbitrary undirected graph containing n vertices and m edges with  $n \le m < 2(n-2)$ . If  $\Delta(G) = n-1$ , then

$$q(G) \le \left(\begin{array}{c} m-n+1\\ 2 \end{array}\right).$$

LEMMA 3.3. [8, A part of Theorem 2.6] Let  $G^{\sigma}$  be an oriented graph with an arc e = (u, v). If e is not contained in any even cycle, then

$$\phi(G^{\sigma},\lambda) = \phi(G^{\sigma} - e,\lambda) + \phi(G^{\sigma} - u - v,\lambda).$$

700



On Oriented Graphs With Minimal Skew Energy

As a consequence of Lemma 3.3, we have the following result.

LEMMA 3.4. Let  $G^{\sigma}$  be an oriented graph on n vertices and (u, v) a pendant arc of  $G^{\sigma}$  with pendant vertex v. Suppose  $\phi(G^{\sigma}, \lambda) = \sum_{i=0}^{n} (-1)^{i} a_{i}(G^{\sigma}) \lambda^{n-i}$ . Then

$$a_i(G^{\sigma}) = a_i(G^{\sigma} - v) + a_{i-2}(G^{\sigma} - v - u).$$

Based on the preliminary results above, we have the following two results.

LEMMA 3.5. Let  $n \geq 5$  and  $G^{\sigma} \in G^{\sigma}(n,m)$  be an oriented graph with maximum degree n-1. Suppose that  $n \leq m < 2(n-2)$  and  $G^{\sigma} \sim O_{n,m}^+$ . Then  $G^{\sigma} \succ O_{n,m}^+$ .

Proof. By Theorem 2.2, it suffices to prove that  $a_4(G^{\sigma}) > a_4(O_{n,m}^+)$ . Suppose that v is the vertex with degree n-1. For convenience, all arcs incident to v are colored as white and all other arcs are colored as black. Then there are n-1 white arcs and m-n+1 black arcs. We estimate the cardinality of 2-matchings in  $G^{\sigma}$  as follows. Noticing that all white arcs are incident to v, each pair of white arc can not form a 2-matching of  $G^{\sigma}$ . Since d(v) = n-1 and each black arc is incident to exactly two white arcs, each black arc together with a white arcs except its neighbors forms a 2-matching of  $G^{\sigma}$ , that is, there are (m-n+1)(n-3) black-white 2-matchings. Moreover, note that  $G^{\sigma} \neq O_{n,m}^+$ ,  $G^{\sigma} - v$  does not contain the directed star  $S_{m-n+2}$ as its subgraph, and thus, there is at least one 2-matching formed by a pair of disjoint black arcs, or  $G^{\sigma}$  is an oriented graph of the following underlying graph F.

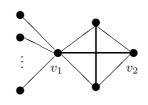


Fig. 3.1. The graph F.

In the former case, the number of 2-matchings in  $G^{\sigma}$  satisfies

$$M(G^{\sigma},2) \ge (m-n+1)(n-3)+1.$$

From Lemma 3.2,  $q(G^{\sigma}) \leq \begin{pmatrix} m-n+1\\ 2 \end{pmatrix}$ , and then by applying Theorem 2.2 again,



S.C. Gong, X.L. Li, and G.H. Xu

we have

$$a_4(G^{\sigma}) \ge M(G^{\sigma}, 2) - 2q(G^{\sigma})$$
  

$$\ge (m - n + 1)(n - 3) + 1 - 2\begin{pmatrix} m - n + 1 \\ 2 \end{pmatrix}$$
  

$$= a_4(O_{n,m}^+) + 1$$

by (3.2). In the latter case, clearly m = n + 2, q(F) = 3, but the three quadrangles can not be all evenly oriented. Then

$$a_4(F) \ge M(F,2) - 2q(F) \ge (m-n+1)(n-3) - 4 > a_4(O_{n,n+2}^+).$$

The result thus follows.  $\square$ 

LEMMA 3.6. Let  $n \geq 5$  and  $G^{\sigma} \in G^{\sigma}(n,m)$  be an oriented graph with  $n \leq m < 2(n-2)$ . Suppose that  $\Delta(G^{\sigma}) \leq n-2$  and  $G^{\sigma} \nsim B^+_{n,m}$ . Then  $G^{\sigma} \succ B^+_{n,m}$ .

*Proof.* By Theorem 2.2 again, it suffices to prove that  $a_4(G^{\sigma}) > a_4(B_{n,m}^+)$ . We prove this inequality by induction on n. By a direct calculation, the result follows if n = 5, since then 5 = m < 2(5 - 2) = 6 and there exists exactly four graphs in  $G^{\sigma}(5,5)$ , namely, the oriented cycle  $C_3$  together with two pendant arcs attached to two different vertices of the  $C_3$ , the oddly oriented cycle  $C_4$  together with a pendant arc,  $B_{5,5}^+$  and the oriented cycle  $C_5$ . Suppose now that  $n \ge 6$  and the result is true for smaller n.

Case 1. There is a pendant arc (u, v) in  $G^{\sigma}$  with pendant vertex v.

By Lemma 3.4 we have

$$a_4(G^{\sigma}) = a_4(G^{\sigma} - v) + a_2(G^{\sigma} - v - u) = a_4(G^{\sigma} - v) + e(G^{\sigma} - v - u).$$

Noticing that  $\Delta(G^{\sigma}) \leq n-2$ , we have  $e(G^{\sigma}-v-u) \geq m-\Delta(G^{\sigma}) \geq m-n+2$ .

By the induction hypothesis,  $a_4(G^{\sigma} - v) \ge a_4(B_{n-1,m-1}^+)$  with equality if and only if  $G^{\sigma} - v = B_{n-1,m-1}^+$ . Then

$$a_4(G^{\sigma}) = a_4(G^{\sigma} - v) + a_2(G^{\sigma} - v - u) \geq a_4(B^+_{n-1,m-1}) + m - n + 2 = a_4(B^+_{n-1,m-1}) + e(S_{m-n+1}) = a_4(B_{n,m})$$

with equality if and only if  $G^{\sigma} = B_{n,m}^+$ . The result thus follows.

Case 2. There are no pendant vertices in  $G^{\sigma}$ .

Let

$$(d)_{G^{\sigma}} = (d_1, d_2, \dots, d_i, d_{i+1}, \dots, d_n)$$



### On Oriented Graphs With Minimal Skew Energy

be the non-increasing degree sequence of  $G^{\sigma}$ . We label the vertices of  $G^{\sigma}$  corresponding to the degree sequence  $(d)_{G^{\sigma}}$  as  $v_1, v_2, \ldots, v_n$  such that  $d_{G^{\sigma}}(v_i) = d_i$  for each *i*. Assume  $d_1 < n-2$ . Then there exists a vertex  $v_k$  that is not adjacent to  $v_1$ , but is adjacent to one neighbor, say  $v_i$ , of  $v_1$ . Thus,

$$(d_1+1, d_2, \ldots, d_i-1, d_{i+1}, \ldots, d_n)$$

is the degree sequence of the oriented graph D' obtained from  $G^{\sigma}$  by deleting the arc  $(v_k, v_i)$  and adding the arc  $(v_k, v_1)$ , regardless the orientation of the arc  $(v_k, v_1)$ . Rewriting the sequence above such that

$$(d)_{D'} = (d'_1, d'_2, \dots, d'_i, d'_{i+1}, \dots, d'_n)$$

is also a non-increasing sequence. Then  $d_1 \ge d_i \ge 2$ , and thus, we have

> 0.

$$\sum_{i=1}^{n} \begin{pmatrix} d'_i \\ 2 \end{pmatrix} > \sum_{i=1}^{n} \begin{pmatrix} d_i \\ 2 \end{pmatrix}, \qquad (3.4)$$

since

702

$$\sum_{i=1}^{n} \begin{pmatrix} d'_{i} \\ 2 \end{pmatrix} - \sum_{i=1}^{n} \begin{pmatrix} d_{i} \\ 2 \end{pmatrix} = \begin{pmatrix} d_{1}+1 \\ 2 \end{pmatrix} + \begin{pmatrix} d_{i}-1 \\ 2 \end{pmatrix} - \begin{pmatrix} d_{1} \\ 2 \end{pmatrix} - \begin{pmatrix} d_{i} \\ 2 \end{pmatrix}$$
$$= d_{1} - d_{i} + 1$$

Repeating this procedure, we can eventually obtain a non-increasing graph sequence

$$(d)_{D''} = (d''_1, d''_2, \dots, d''_i, d''_{i+1}, \dots, d''_n)$$

such that  $\Delta(D'') = d''_1 = n - 2$  and

$$\sum_{v \in D''} \begin{pmatrix} d''(v) \\ 2 \end{pmatrix} > \sum_{v \in D'} \begin{pmatrix} d'(v) \\ 2 \end{pmatrix} > \dots > \sum_{v \in G^{\sigma}} \begin{pmatrix} d(v) \\ 2 \end{pmatrix}.$$
 (3.5)

Similarly, we can assume that there exists a vertex  $v_k$  that is not adjacent to  $v_i$ , but is adjacent to one neighbor, say  $v_j$ , of  $v_i$ . Thus,

$$(d_1, d_2, \dots, d_i + 1, d_{i+1}, \dots, d_j - 1, d_{j+1}, \dots, d_n)$$

is the degree sequence of the oriented graph D''' obtained from D'' by deleting the arc  $(v_k, v_j)$  and inserting the arc  $(v_k, v_i)$ , regardless the orientation of the arc  $(v_k, v_j)$ . By a similar proof, we can get

$$\sum_{v \in D'''} \begin{pmatrix} d'''(v) \\ 2 \end{pmatrix} > \sum_{v \in D''} \begin{pmatrix} d''(v) \\ 2 \end{pmatrix}.$$

703

S.C. Gong, X.L. Li, and G.H. Xu

By repeatedly applying the above procedure, we eventually obtain the degree sequence  $(d)_{B_n^+ m}$ ,

$$(d)_{B_{n,m}^+} = (n-2, m-n+2, 2, 2, \dots, 2, 1, 1, \dots, 1),$$

where the number of vertices of degree 2 is m - n + 2, and the number of vertices of degree 1 is 2n - m - 4. Finally, we get

$$\sum_{v \in B_{n,m}^+} \begin{pmatrix} d^{B^+}(v) \\ 2 \end{pmatrix} > \sum_{v \in D^{\prime\prime\prime}} \begin{pmatrix} d^{\prime\prime\prime}(v) \\ 2 \end{pmatrix} > \sum_{v \in D^{\prime\prime}} \begin{pmatrix} d^{\prime\prime}(v) \\ 2 \end{pmatrix} > \dots > \sum_{v \in G^{\sigma}} \begin{pmatrix} d(v) \\ 2 \end{pmatrix}.$$

Then the lemma follows by combining (3.3) and Lemma 3.1 with the fact that  $M(G,2) = \binom{m}{2} - \sum_{v \in G^{\sigma}} \binom{d(v)}{2}$ .

Combining Lemma 3.5 with Lemma 3.6, we get the proof of Theorem 1.1 immediately.

Proof of Theorem 1.1. Combining with Lemmas 3.5 and 3.6, the oriented graph with minimal skew energy among all oriented graphs of  $G^{\sigma}(n,m)$  with  $n \leq m \leq 2(n-2)$  is either  $O_{n,m}^+$  or  $B_{n,m}^+$ . Furthermore, from (3.2) and (3.3), we have

$$a_4(O_{n,m}^+) = (m-n+1)(2n-m-3)$$

and

$$a_4(B_{n,m}^+) = (m-n+2)(2n-m-4).$$

Then, by a direct calculation we have  $a_4(O_{n,m}^+) < a_4(B_{n,m}^+)$  if  $m < \frac{3n-5}{2}$ ,  $a_4(B_{n,m}^+) = a_4(O_{n,m}^+)$  if  $m = \frac{3n-5}{2}$ , and  $a_4(O_{n,m}^+) > a_4(B_{n,m}^+)$  otherwise. The proof is thus complete by (3.1).  $\Box$ 

# REFERENCES

- C. Adiga, R. Balakrishnan, and W. So. The skew energy of a graph. Linear Algebra Appl., 432:1825–1835. 2010.
- [2] F. Alinaghipour and B. Ahmadi. On the energy of complement of regular line graph. MATCH Commun. Math. Comput. Chem., 60:427–434, 2008.
- [3] S. Akbari, E. Ghorbani, and M.R. Oboudi. Edge addition, singular values and energy of graphs and matrices. *Linear Algebra Appl.*, 430:2192–2199, 2009.
- S.R. Blackburn and I.E. Shparlinski. On the average energy of circulant graphs. *Linear Algebra Appl.*, 428:1956–1963, 2008.
- [5] G. Caporossi, D. Cvetković, I. Gutman, and P. Hansen. Variable neighborhood search for extremal graphs. 2. Finding graphs with external energy. J. Chem. Inf. Comput. Sci., 39:984–996, 1999.

704



#### On Oriented Graphs With Minimal Skew Energy

- [6] C.A. Coulson. On the calculation of the energy in unsaturated hydrocarbon molecules. Proc. Cambridge Phil. Soc., 36:201–203, 1940.
- [7] J. Day and W. So. Graph energy change due to edge deletion. *Linear Algebra Appl.*, 428:2070–2078, 2007.
- [8] S. Gong and G. Xu. The characteristic polynomial and the matchings polynomial of a weighted oriented graph. *Linear Algebra Appl.*, 436:3597–3607, 2012.
- [9] S. Gong and G. Xu. 3-Regular digraphs with optimum skew energy. Linear Algebra Appl., 436:465–471, 2012.
- [10] I. Gutman. The energy of a graph. Ber. Math.-Statist. Sekt. Forschungsz. Graz., 103:1–22, 1978.
- [11] I. Gutman. The energy of a graph: Old and new results. In: A. Betten, A. Kohnert, R. Laue, and A. Wassermann (editors), *Algebraic Combinatorics and Applications*, Springer, Berlin, 196–211, 2000.
- [12] I. Gutman, D. Kiani, and M. Mirzakhah. On incidence energy of graphs. MATCH Commun. Math. Comput. Chem., 62:573–580, 2009.
- [13] I. Gutman, D. Kiani, M. Mirzakhah, and B. Zhou. On incidence energy of a graph. *Linear Algebra Appl.*, 431:1223–1233, 2009.
- [14] I. Gutman and O.E. Polansky. Mathematical Concepts in Organic Chemistry, Springer, Berlin, 1986.
- [15] I. Gutman, M. Robbiano, E.A. Martins, D.M. Cardoso, L. Medina, and O. Rojo. Energy of line graphs. *Linear Algebra Appl.*, 433:1312–1323, 2010.
- [16] I. Gutman and B. Zhou. Laplacian energy of a graph. Linear Algebra Appl., 414:29-37, 2006.
- [17] Y. Hou. Unicyclic graphs with minimal energy. J. Math. Chem., 29:163–168, 2001.
- [18] Y. Hou. Bicyclic graphs with minimum energy. Linear Multilinear Algebra, 49:347–354, 2001.
- [19] Y. Hou and T. Lei. Characteristic polynomials of skew-adjacency matrices of oriented graphs. *Electron. J. Combin.*, 18:Article 156, 2011.
- [20] Y. Hou, X. Shen, and C. Zhang. Oriented unicyclic graphs with extremal skew energy. Preprint, available at http://arXiv.org/abs/1108.6229.
- [21] X. Li, Y. Shi, and I. Gutman. Graph Energy, Springer, New York, 2012.
- [22] X. Li, J. Zhang, and L. Wang. On bipartite graphs with minimal energy. Discrete Appl. Math., 157:869–873, 2009.
- [23] X. Shen, Y. Hou, and C. Zhang. Bicyclic digraphs with extremal skew energy. Electron. J. Linear Algebra, 23:340–355, 2012.
- [24] G. Tian. On the skew energy of orientations of hypercubes. Linear Algbra Appl., 435:2140–2149, 2011.
- [25] J. Zhang and B. Zhou. On bicyclic graphs with minimal energies. J. Math. Chem., 37(4):423– 431, 2005.
- [26] J. Zhu. Oriented unicyclic graphs with the first  $\lfloor \frac{n-9}{2} \rfloor$  largest skew energies. Linear Algebra Appl., 437:2630–2649, 2012.