

## On tricyclic graphs with minimal energy\*

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**Abstract.** The energy of a graph is defined as the sum of the absolute values of all the eigenvalues of the graph. Let  $\mathcal{G}_n$  be the class of tricyclic graphs  $G$  on  $n$  vertices and containing no disjoint odd cycles  $C_p, C_q$  of lengths  $p$  and  $q$  with  $p+q \equiv 2 \pmod{4}$ . In this paper, we obtain the minimal and second-minimal values on the energies of the graphs in  $\mathcal{G}_n$  and determine the corresponding graphs.

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### 1. Introduction

Let  $G$  be a simple graph with  $n$  vertices. Let  $A(G)$  be the adjacency matrix of  $G$ . The characteristic polynomial of  $G$  is

$$\phi(G, \lambda) = \det(\lambda I - A) = \sum_{i=0}^n a_i \lambda^{n-i},$$

Sachs theorem states that [12] for  $i \geq 1$ ,

$$a_i = \sum_{S \in L_i} (-1)^{p(S)} 2^{c(S)},$$

where  $L_i$  denotes the set of Sachs graphs of  $G$  with  $i$  vertices, that is, the graphs in which every component is either a  $K_2$  or a cycle,  $p(S)$  is the number of components of  $S$  and  $c(S)$  is the number of cycles contained in  $S$ . In addition  $a_0 = 1$ . The roots  $\lambda_1, \dots, \lambda_n$  of  $\phi(G, \lambda)$  are called the eigenvalues of  $G$ . Since  $A(G)$  is symmetric, all eigenvalues of  $G$  are real. Let  $C_n$  denote a cycle of length  $n$ . Other undefined notation may refer to [2, 12].

The energy of  $G$ , denoted by  $E(G)$ , is then defined as  $E(G) = \sum_{i=1}^n |\lambda_i|$ . Since the energy of a graph can be used to approximate the total  $\pi$ -electron energy of the molecule (e.g., see [11, 12]), there are numerous results on  $E(G)$  (e.g., see [1,3,4,5-11,13-27,29-33,35-42]), including graphs with extremal energies [3,7,17,18,20,21,23-26,30,31,33,35-40,43-47].

It is known that [12]  $E(G)$  can be expressed as the Coulson integral formula

$$E(G) = \frac{1}{\pi} \int_0^{+\infty} \frac{dx}{x^2} \ln \left[ \left( \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^i a_{2i} x^{2i} \right)^2 + \left( \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^i a_{2i+1} x^{2i+1} \right)^2 \right]. \quad (1.1)$$

Let  $b_{2i}(G) = (-1)^i a_{2i}$  and  $b_{2i+1}(G) = (-1)^i a_{2i+1}$  for  $0 \leq i \leq \lfloor \frac{n}{2} \rfloor$ . Clearly,  $b_0(G) = 1$  and  $b_2(G)$  equals the number of edges of  $G$ . Thus, by (1.1),  $E(G)$  is a strictly monotonically increasing function of  $b_i(G)$ ,  $i = 1, \dots, \lfloor n/2 \rfloor$ . A quasi-order is introduced (see [12]): if  $G_1$  and  $G_2$  are two graphs, then

$$G_1 \succeq G_2 \Leftrightarrow b_i(G_1) \geq b_i(G_2) \text{ for all } i \geq 0.$$

If  $G_1 \succeq G_2$ , and there exists one  $j$  such that  $b_j(G_1) > b_j(G_2)$ , then we write  $G_1 \succ G_2$ . Therefore,

$$G_1 \succ G_2 \Rightarrow E(G_1) > E(G_2).$$

Many results on the minimal energy have been obtained for various classes of graphs. In [3], Caporossi et al. gave the following conjecture.

**Conjecture 1.1.** *Connected graphs  $G$  with  $n \geq 6$  vertices,  $n - 1 \leq e \leq 2(n - 2)$  edges and minimum energy are star with  $e - n + 1$  additional edges all connected to the same vertex for  $e \leq n + \lfloor \frac{n-7}{2} \rfloor$ , and bipartite graphs with two vertices on one side, one of which is connected to all vertices on the other side otherwise.*

This conjecture is true when  $e = n - 1, 2(n - 2)$  [3, Theorem 1], and when  $e = n$  for  $n \geq 6$  [17],  $e = n + 1$  for  $n \geq 9$  [39]. In this paper, we consider the above conjecture for the case  $e = n + 2$  for  $n \geq 7$ .



Figure 1: Graphs  $G_n^0$  and  $G_n^1$

A connected simple graph with  $n$  vertices and  $e = n + 2$  edges is called a *tricyclic graph*. Let  $\mathcal{G}_n$  be the class of tricyclic graph  $G$  with  $n$  vertices and containing no disjoint two odd cycles  $C_p, C_q$  with  $p + q \equiv 2 \pmod{4}$ . Let  $G_n^0$  be the graph formed by joining 3 pendent vertices to a vertex of degree one of the  $K_{1,n-1}$  (e.g., see Figure 1), and  $G_n^1$  be the graph formed by joining  $n - 6$  pendent vertices to a vertex of degree 4 of the complete bipartite graph  $K_{2,4}$  (e.g., see Figure 1). In this paper, we show that  $G_n^0, G_n^1$  have, respectively, minimal and the second-minimal energies in  $\mathcal{G}_n$  for  $n \geq 11$  and  $G_n^1$  has the minimal energy in  $\mathcal{G}_n$  for  $7 \leq n \leq 10$ .

The following two lemmas are needed in our paper.

**Lemma 1.2** ([39]). *Let  $G$  be a graph with  $n$  vertices and let  $uv$  be a pendent edge of  $G$  with pendent vertex  $v$ . Then for  $2 \leq i \leq n$ ,  $b_i(G) = b_i(G - v) + b_{i-2}(G - u - v)$ .*

**Lemma 1.3** ([39]). *Let  $G$  be any graph. Then  $b_4(G) = m(G, 2) - 2s$ , where  $m(G, 2)$  is the number of 2-matchings of  $G$  and  $s$  is the number of quadrangles in  $G$ .*

**2. Lemmas and main results**

In this section, we shall determine the tricyclic graphs in  $\mathcal{G}_n$  ( $n \geq 11$ ) having the minimal and the second-minimal energies. Our idea is, at first, to show  $E(G) > E(G_n^1)$  for any  $G \in \mathcal{G}_n$  with  $G \not\cong G_n^0, G_n^1, R_n, W_n, S_n, Q_n$ ; and proceed to show that  $E(G_n^0) < E(G_n^1)$ , where  $R_n, S_n, Q_n$  are as shown in Figure 2. For  $\mathcal{G}_n$  with  $7 \leq n \leq 10$ , we characterize the graph with minimal energy. The following fact is immediate.

**Fact 1.** *For any  $G \in \mathcal{G}_n$ , there are at most three edge-disjoint cycles contained in  $G$ .*

**Lemma 2.1.** *If  $G \in \mathcal{G}_n$ , then  $b_{2i} \geq 0$  for  $0 \leq i \leq \lfloor \frac{n}{2} \rfloor$ .*

*Proof.* Let  $L_i$  be the set of Sachs graphs of  $G$  with  $i$  vertices. By Sachs theorem,

$$b_{2i} = \sum_{S \in L_{2i}} (-1)^{p(S)+i} 2^{c(S)} = \sum_{S \in L_{2i}^1} (-1)^{p(S)+i} + \sum_{S \in L_{2i}^2} (-1)^{p(S)+i} 2^{c(S)},$$

where  $L_{2i}^1$  is the set of graphs with no cycles in  $L_{2i}$ , and  $L_{2i}^2 = L_{2i} \setminus L_{2i}^1$ .

If every  $S$  in  $L_{2i}$  has no cycle, then  $p(S) = i$ , and so

$$b_{2i}(G) = \sum_{S \in L_{2i}} 1 \geq 0.$$

Otherwise, there exists  $S'$  in  $L_{2i}$  such that  $S'$  contains cycles. If  $S'$  has no odd cycles, then  $b_{2i}(G) \geq 0$  [14]; otherwise, together with Fact 1,  $S'$  must contain two edge-disjoint odd cycles, say  $C_k, C_l$ . Since  $G \in \mathcal{G}_n$ , we have  $k + l \equiv 0 \pmod{4}$ . If  $S'$  has no cycle except  $C_k$  and  $C_l$ , then

$$p(S') + i = 2 + \frac{2i - (k + l)}{2} + i \equiv 0 \pmod{2}.$$

If  $S'$  has another cycle  $C_m$ , then  $C_m$  must be even. Thus its corresponding term in  $b_{2i}$  is the following

$$(-1)^{p(S')+i} 2^3.$$

On the other hand, since  $C_m$  is an even cycle, it has exactly two perfect matching, say  $M_1, M_2$ , therefore there exist Sachs graphs  $S_1'', S_2''$  in  $L_{2i}$  such that  $S_1'' := (S' \setminus C_m) \cup C_k \cup C_l \cup M_1$  and  $S_2'' := (S' \setminus C_m) \cup C_k \cup C_l \cup M_2$ , respectively. Its corresponding term in  $b_{2i}$  is the following

$$(-1)^{p(S_1'')+i} \cdot 2^2 + (-1)^{p(S_2'')+i} \cdot 2^2,$$

where  $p(S_1'') + i = p(S_2'') + i = 2 + \frac{2i - (k+l)}{2} + i \equiv 0 \pmod{2}$ . It is easy to see  $|L_{2i}^2| \geq 2|L_{2i}^1|$ , and so

$$b_{2i} \geq \sum_{\substack{C_m \subseteq S' \in L_{2i}^2 \\ M_1, M_2 \subseteq C_m}} \left[ (-1)^{p(S_1'')+i} \cdot 2^2 + (-1)^{p(S_2'')+i} \cdot 2^2 + (-1)^{p(S'')+i} \cdot 2^3 \right] \geq 0,$$

where  $S_1'' = (S' \setminus C_m) \cup C_k \cup C_l \cup M_1$  and  $S_2'' = (S' \setminus C_m) \cup C_k \cup C_l \cup M_2$ . □

In  $\mathcal{G}_n$ , there exist four special graphs, namely that  $R_n, W_n, S_n, Q_n$ ; see Figure 2, where  $R_n$  has  $n - 7$  pendent vertices,  $W_n$  has  $n - 6$  pendent vertices,  $S_n$  has  $n - 5$  pendent vertices and  $Q_n$  has  $n - 4$  pendent vertices. In the following lemmas, we shall repeatedly use these graphs.

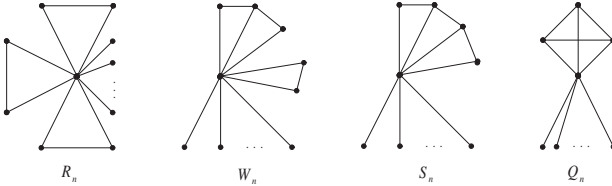


Figure 2: Graphs  $R_n, W_n, S_n$  and  $Q_n$ .

It is straightforward to check that graph  $G \in \mathcal{G}_n$  has at least 3 cycles and at most 7 cycles. Furthermore, there do not exist five cycles in  $G$ .

Let  $m(G, 2)$  denote the number of 2-matchings of a graph  $G$ . Obviously,  $m(P_n, 2) = (n - 2)(n - 3)/2$  and  $m(C_n, 2) = n(n - 3)/2$ .

**Lemma 2.2.** *If  $G \in \mathcal{G}_n$  has exactly three cycles with  $G \not\cong R_n$ , then  $b_4(G) > b_4(G_n^1)$  for  $n \geq 7$ .*

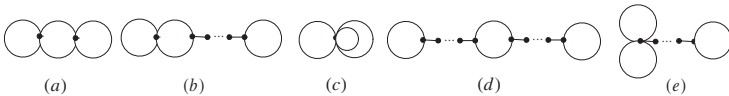


Figure 3: Five possible cases for the arrangement of three cycles in  $G$ .

*Proof.* Since  $G \in \mathcal{G}_n$  contains exactly three cycles, say  $C_a, C_b, C_c$ , then these must be edge-disjoint; see Figure 3. It is immediate that  $n + 2 - a - b - c \geq 0$ . By induction on  $n + 2 - a - b - c$ . If  $n + 2 - a - b - c = 0$ , then either  $C_a, C_b, C_c$  has exactly one vertex in common (e.g., see (c) in Figure 3), or there exist two pairs of cycles in  $\{C_a, C_b, C_c\}$ , such that each pair of cycles, say  $\{C_a, C_b\}$  (respectively,  $\{C_b, C_c\}$ ) have a vertex in common, say  $v_1$  (respectively,  $v_2$ ) satisfying  $v_1 \neq v_2$  (e.g., see (c) in Figure 3). For the latter, by Lemma 1.2, we have

$$\begin{aligned} b_4(G) &= m(G, 2) - 2s \geq m(G, 2) - 6 \\ &= \frac{a(a-3)}{2} + \frac{b(b-3)}{2} + \frac{c(c-3)}{2} + (a-2)(n+2-a) \\ &\quad + 2(n+2-a-2) + (b-2)c + 2(c-2) - 6 \\ &= \frac{1}{2}(a+b+c)^2 - \frac{3}{2}(a+b+c) - 14 \\ &= \frac{1}{2}n^2 + \frac{1}{2}n - 15. \end{aligned}$$

and so

$$b_4(G) - b_4(G_n^1) \geq \frac{1}{2}n^2 + \frac{1}{2}n - 15 - (4n - 24) = \frac{1}{2}n^2 - \frac{7}{2}n + 9 > 0,$$

and hence  $b_4(G) > b_4(G_n^1)$ . Similarly, for the former, namely that for (c) in Figure 3, we can also prove  $b_4(G) > b_4(G_n^1)$  when  $p = k \geq 1$ .

Suppose it is true for all graphs  $G \in \mathcal{G}_n$  having exactly three cycles and  $G \not\cong R_n$  with  $n + 2 - a - b - c < p$  ( $p \geq 1$ ), and suppose  $n + 2 - a - b - c = p$ .

*Case 1.* There are no pendent edges in  $G$ . Then there are at most two cycles having a vertex in common.

*Subcase 1.1.* If there are exactly two cycles, say  $C_b$  and  $C_c$ , having exactly one vertex in common; see (b), (e) in Figure 3. For (b) in Figure 3, if  $p = k \geq 1$ , then  $C_b$  (or,  $C_c$ ) connects  $C_a$  by a path of length  $k$ . Without loss of generality, let  $C_b$  connect  $C_a$  by a path of length  $k$ . By Lemma 1.2,

$$\begin{aligned} b_4(G) &= m(G, 2) - 2s \geq m(G, 2) - 6 \\ &= \frac{a(a-3)}{2} + \frac{b(b-3)}{2} + \frac{c(c-3)}{2} + \frac{(k-1)(k-2)}{2} + (a-2)(n+2-a) \\ &\quad + 2(n+2-a-1) + (k-1)(b+c) + (b-2+c) \end{aligned}$$

$$\begin{aligned}
 & +(b-2)c + 2(c-2) - 6 \\
 = & \frac{1}{2}(a+b+c)^2 - \frac{3}{2}(a+b+c) + k(a+b+c) + \frac{(k-1)(k-2)}{2} - 14 \\
 = & \frac{1}{2}n^2 + \frac{1}{2}n - 14,
 \end{aligned}$$

and thus

$$b_4(G) - b_4(G_n^1) \geq \frac{1}{2}n^2 + \frac{1}{2}n - 14 - (4n - 24) = \frac{1}{2}n^2 + \frac{7}{2}n + 10 > 0,$$

and therefore  $b_4(G) > b_4(G_n^1)$ . Similarly, for the former, namely that for (e) in Figure 1, we can also prove  $b_4(G) > b_4(G_n^1)$  when  $p = k \geq 1$ .

*Subcase 1.2* If there does not exist two cycles in  $\{C_a, C_b, C_c\}$  having exactly one vertex in common, then set  $n + 2 - a - b - c = k \geq 2$ . Hence there exist two pairs of cycles in  $\{C_a, C_b, C_c\}$ , say  $\{C_a, C_b\}$  and  $\{C_b, C_c\}$ , such that each pair of such two cycles are connected by a path. Without loss of generality, assume that  $C_a$  (respectively,  $C_c$ ) connects  $C_b$  by  $P_{r+1}$  (respectively,  $P_{l+1}$ ), where  $r \geq 1$  (respectively,  $l \geq 1$ ). Then by Lemma 1.2,

$$\begin{aligned}
 b_4(G) & = m(G, 2) - 2s \geq m(G, 2) - 6 \\
 & = \frac{a(a-3)}{2} + \frac{b(b-3)}{2} + \frac{c(c-3)}{2} + \frac{(r-1)(r-2)}{2} + \frac{(l-1)(l-2)}{2} \\
 & + (a-2)(n+2-a) + 2(n+2-a-1) + (r-1)(b+c+l) - 6 \\
 & + (b+c+l-2) + (b-2)(c+l) + 2(c+l-1) + (l-1)c + (c-2) \\
 & = \frac{1}{2}(a+b+c)^2 - \frac{3}{2}(a+b+c) + k(a+b+c) + \frac{1}{2}(k-2)(k-3) - 15 \\
 & = \frac{1}{2}n^2 + \frac{1}{2}n - 13,
 \end{aligned}$$

and so

$$b_4(G) - b_4(G_n^1) \geq \frac{1}{2}n^2 + \frac{1}{2}n - 13 - (4n - 24) = \frac{1}{2}n^2 - \frac{7}{2}n + 11 > 0.$$

It is immediate that  $b_4(G) > b_4(G_n^1)$ .

*Case 2.*  $uv$  is a pendent edge of  $G$  with pendent vertex  $v$ . By Lemma 1.1,

$$b_4(G) = b_4(G-v) + b_2(G-u-v), \quad b_4(G_n^1) = b_4(G_{n-1}^1) + b_2(K_{1,4}).$$

Note that  $G - v$  has exactly three cycles on  $n - 1$  vertices and  $G \not\cong R_n$ , therefore  $G - v \not\cong G_{n-1}^0, G_{n-1}^1, W_{n-1}, S_{n-1}, Q_{n-1}, R_{n-1}$ , by induction hypothesis,  $b_4(G - v) > b_4(G_{n-1}^1)$ . It is easy to see  $G \not\cong G_n^0, G_n^1, W_n, S_n, Q_n, R_n$ , we have  $b_2(G - u - v) \geq b_2(K_{1,4}) = 4$ . It is immediate that  $b_4(G) > b_4(G_n^1)$  with  $G \not\cong R_n$ .

By combing Cases 1 and 2, this lemma follows. □

**Remark.** In Case 2 above, if  $G \cong R_n$ , then  $b_2(G - u - v) = 3 < b_2(K_{1,4}) = 4$ . This is just the reason why we consider  $G \in \mathcal{G}_n$  with  $G \not\cong R_n$ .

**Lemma 2.3.** *If  $G \in \mathcal{G}_n$  has exactly four cycles with  $G \not\cong W_n$ , then  $b_4(G) > b_4(G_n^1)$  for  $n \geq 7$ .*

*Proof.* Since  $G$  has exactly four cycles, by Fact 1, there are two cycles, say  $C_a$  and  $C_b$ , having  $t$  ( $t \geq 1$ ) common edges and there exists exactly one cycle, say  $C_c$ , which is edge-disjoint with the rest cycles contained in  $G$  (e.g., see Figure 4.). So  $n + 2 - a - b + t - c \geq 0$ . By induction on  $n + 2 - a - b + t - c$ . If  $n + 2 - a - b + t - c = 0$ , then either all of the four cycles have a vertex in common, or there exists exactly one cycle, say  $C_b$ , connecting  $C_c$  by a vertex, that is, only  $C_b$  and  $C_c$  have exactly one vertex in common.

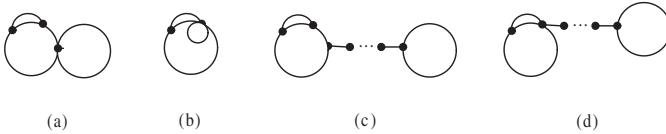


Figure 4: Four possible cases for the arrangement of four cycles in  $G$

When  $t = 1$ , by Lemma 1.2,

$$\begin{aligned}
 b_4(G) &= m(G, 2) - 2s \geq m(G, 2) - 8 \\
 &= \frac{(a + b - 2)(a + b - 5)}{2} + \frac{c(c - 3)}{2} + (a + b - 2 - 4 + c) \\
 &\quad + (a + b - 2 - 2)c + 2(c - 2) - 8 \\
 &= \frac{(a + b)^2}{2} - \frac{5}{2}(a + b) + (a + b)c + \frac{c^2 - 5c}{2} - 13.
 \end{aligned}$$



Since  $n + 2 - a - b + 1 - c = 0$ , thus  $a + b = n + 3 - c$ . And so

$$\begin{aligned} b_4(G) - b_4(G_n^1) &\geq \frac{(n + 3 - c)^2}{2} - \frac{5}{2}(n + 3 - c) + (n + 3 - c)c + \frac{c^2 - 5c}{2} \\ &\quad - 13 - (4n - 24) \\ &= \frac{1}{2}n^2 - \frac{7}{2}n + 8 > 0, \end{aligned}$$

and hence  $b_4(G) > b_4(G_n^1)$ .

When  $t \geq 2$ , by Lemma 1.2,

$$\begin{aligned} b_4(G) &= m(G, 2) - 2s \geq m(G, 2) - 8 \\ &= \frac{(a + b - 2t)(a + b - 2t - 3)}{2} + \frac{c(c - 3)}{2} + \frac{(t - 1)(t - 2)}{2} + 2(c - 2) - 8 \\ &\quad + 2(a + b - 2t - 2 + c) + (t - 2)(a + b - 2t + c) + (a + b - 2t - 2)c \\ &= \frac{(a + b)^2}{2} - (t + \frac{3}{2})(a + b) + (a + b)c + \frac{c^2 - 3c}{2} + \frac{(t - 1)(t - 2)}{2} \\ &\quad + 3t - tc - 16. \end{aligned}$$

Since  $n + 2 - a - b + t - c = 0$ , thus  $a + b = n + 2 + t - c$ . And so

$$b_4(G) - b_4(G_n^1) \geq \begin{cases} \frac{1}{2}n^2 - \frac{7}{2}n + 14, & \text{if } t = 2; \\ \frac{1}{2}n^2 - \frac{7}{2}n + 8, & \text{if } t \geq 3. \end{cases}$$

and therefore  $b_4(G) > b_4(G_n^1)$  for  $n \geq 7$ . Similarly, in the case that all of the four cycles have exactly one vertex in common when  $n \geq 7$ , the result  $b_4(G) > b_4(G_n^1)$  also holds for  $n + 2 - a - b + t - c = 0$ .

Suppose it is true for all graphs  $G \in \mathcal{G}_n$  having exactly four cycles and  $G \not\cong W_n$  with  $n + 2 - a - b + t - c < p$  ( $p \geq 1$ ), and suppose  $n + 2 - a - b + t - c = p$ .

*Case 1.* There is no pendent edges in  $G$ . Then either there exactly one cycle, say  $C_b$ , connecting the separated cycle, say  $C_c$ , by a path of length  $p$ , or the separated cycle connects the rest three cycles by a path of length  $p$ , that is, one end vertex of this path is in the separated cycle, the other end vertex is a common vertex of the rest cycles. Here we show our result only for the former, similarly we can prove our result for the latter case.

*Subcase 1.1.*  $t = 1$ . Then by Lemma 1.2,

$$\begin{aligned} b_4(G) &= m(G, 2) - 2s \geq m(G, 2) - 8 \\ &= \frac{(a+b-2)(a+b-5)}{2} + \frac{c(c-3)}{2} + \frac{(p-1)(p-2)}{2} + (a+b-2-2) - 8 \\ &\quad + (a+b-2)(c+p-1) + (a+b-2-4+c+p) + (p-1)c + (c-2) \\ &= \frac{(a+b)^2}{2} - \frac{5}{2}(a+b) + (a+b)(c+p) + \frac{c^2-5c}{2} + \frac{p^2-5p}{2} + pc - 12. \end{aligned}$$

Since  $n+2-a-b+1-c=p$ , we  $a+b=n+3-p-c$ . And so

$$\begin{aligned} b_4(G) - b_4(G_n^1) &\geq \frac{(n+3-p-c)^2}{2} - \frac{5}{2}(n+3-p-c) + (n+3-p-c)(c+p) \\ &\quad + \frac{c^2-5c}{2} + \frac{p^2-5p}{2} + pc - 12 - (4n-24) \\ &= \frac{1}{2}n^2 - \frac{7}{2}n + 9 > 0, \end{aligned}$$

and thereby  $b_4(G) > b_4(G_n^1)$ .

*Subcase 1.2.*  $t = 2$ . Then by Lemma 1.2,

$$\begin{aligned} b_4(G) &= m(G, 2) - 2s \geq m(G, 2) - 8 \\ &= \frac{(a+b-4)(a+b-7)}{2} + \frac{c(c-3)}{2} + \frac{(p-1)(p-2)}{2} + 2(a+b-4-2+c+p) \\ &\quad + (a+b-4-2)(c+p) + 2(c+p-1) + (p-1)c + (c-2) - 8 \\ &= \frac{(a+b)^2}{2} - \frac{7}{2}(a+b) + (a+b)(c+p) + \frac{c^2-7c}{2} + \frac{p^2-7p}{2} + pc - 9. \end{aligned}$$

Since  $n+2-a-b+2-c=p$ , we have  $a+b=n+4-c-p$ . And so

$$\begin{aligned} b_4(G) - b_4(G_n^1) &\geq \frac{(n+4-c-p)^2}{2} - \frac{7}{2}(n+4-c-p) + (n+4-c-p)(c+p) \\ &\quad + \frac{c^2-7c}{2} + \frac{p^2-7p}{2} + pc - 9 - (4n-24) \\ &= \frac{1}{2}n^2 - \frac{7}{2}n + 9 > 0, \end{aligned}$$

and hence  $b_4(G) > b_4(G_n^1)$ .

*Subcase 1.3.*  $t \geq 3$ . Then by Lemma 1.2,

$$\begin{aligned} b_4(G) &= m(G, 2) - 2s \geq m(G, 2) - 8 \\ &= \frac{(a+b-2t)(a+b-2t-3)}{2} + \frac{c(c-3)}{2} + \frac{(t-1)(t-2)}{2} + \frac{(p-1)(p-2)}{2} \\ &\quad + 2(a+b-2t-2+c+p) + (t-2)(a+b-2t+c+p) \\ &\quad + (a+b-2t-2)(c+p) + 2(c+p-1) + (p-1)c + (c-2) - 8 \end{aligned}$$

$$= \frac{(a+b)^2}{2} - (t + \frac{3}{2})(a+b) + (a+b)(c+p) + \frac{c^2 - 3c}{2} + \frac{t^2 + 3t}{2} + \frac{p^2 - 3p}{2} + pc - tc - pt - 14.$$

Since  $n + 2 - a - b + t - c = p$ , we have  $a + b = n + 2 + t - c - p$ . And so

$$\begin{aligned} b_4(G) - b_4(G_n^1) &\geq \frac{(n + 2 + t - c - p)^2}{2} - (t + \frac{3}{2})(n + 2 + t - c - p) \\ &\quad + (n + 2 + t - c - p)(c + p) + \frac{c^2 - 3c}{2} + \frac{t^2 + 3t}{2} + \frac{p^2 - 3p}{2} \\ &\quad + pc - tc - pt - 14 - (4n - 24). \\ &= \frac{1}{2}n^2 - \frac{7}{2}n + 9 > 0, \end{aligned}$$

and therefore  $b_4(G) > b_4(G_n^1)$ .

*Subcase 2.*  $uv$  is a pendent edge of  $G$  with pendent vertex  $v$ . By Lemma 1.1,

$$b_4(G) = b_4(G - v) + b_2(G - u - v), \quad b_4(G_n^1) = b_4(G_{n-1}^1) + b_2(K_{1,4}).$$

Note that  $G - v$  has exactly four cycles on  $n - 1$  vertices and  $G \not\cong W_n$ , therefore  $G - v \not\cong G_{n-1}^0, G_{n-1}^1, R_{n-1}, S_{n-1}, Q_{n-1}, W_{n-1}$ , by induction hypothesis,  $b_4(G - v) > b_4(G_{n-1}^1)$ . It is easy to see  $G \not\cong G_n^0, G_n^1, W_n, S_n, Q_n, R_n$ , we have  $b_2(G - u - v) \geq b_2(K_{1,4}) = 4$ . It is immediate that  $b_4(G) > b_4(G_n^1)$  with  $G \not\cong W_n$ .

By combing Cases 1 and 2, this lemma follows. □

**Lemma 2.4.** *If  $G \in \mathcal{G}_n$  has exactly six cycles and  $G \not\cong G_n^0, G_n^1, S_n$ , then  $b_4(G) > b_4(G_n^1)$  for  $n \geq 7$ .*

*Proof.* Since  $G$  has six cycles, then it is straightforward to check that either any two of the six cycles have exactly two vertices in common, or there are two cycles either having exactly one vertex in common, or having no vertex in common; see Figure 5.

*Case 1.* Any two of the six cycles have exactly two vertices in common. Thus choose three cycles  $C_a, C_b$  and  $C_c$  having  $t$  edges in common. Then  $n + 2 - a - b - c + 2t \geq 0$ . By induction on  $n + 2 - a - b - c + 2t$ . Assume  $n + 2 - a - b - c + 2t = 0$ ,

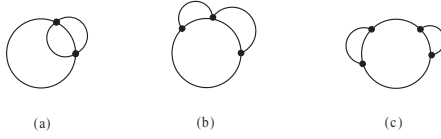


Figure 5: Three possible cases for the arrangement of six cycles in  $G$

When  $t = 1$ , by Lemma 1.2,

$$\begin{aligned}
 b_4(G) &= m(G, 2) - 2s \geq m(G, 2) - 12 \\
 &= \frac{(a+b-2)(a+b-5)}{2} + \frac{c(c-3)}{2} + (a+b-2-4) \\
 &\quad + 2(a+b-2-2) + (c-3)(a+b-2) - 12 \\
 &= \frac{(a+b)^2}{2} - \frac{7}{2}(a+b) + (a+b)c + \frac{c^2-7c}{2} - 15.
 \end{aligned}$$

Since  $n+2-a-b+2-c=0$ , we have  $a+b=n+4-c$ . And so

$$\begin{aligned}
 b_4(G) - b_4(G_n^1) &\geq \frac{(n+4-c)^2}{2} - \frac{7}{2}(n+4-c) + (n+4-c)c + \frac{c^2-7c}{2} \\
 &\quad - 15 - (4n-24) \\
 &= \frac{1}{2}n^2 - \frac{7}{2}n + 3,
 \end{aligned}$$

and hence  $b_4(G) > b_4(G_n^1)$  for  $n \geq 7$ .

When  $t = 2$ . Let  $c = 2 + l$ , if  $l = 1$ , by Lemma 1.2,

$$\begin{aligned}
 b_4(G) &= m(G, 2) - 2s \geq m(G, 2) - 12 \\
 &= \frac{(a+b-4)(a+b-7)}{2} + \frac{c(c-3)}{2} + 2(a+b-4-2) + (a+b-4-4) - 12 \\
 &= \frac{(a+b)^2}{2} - \frac{5}{2}(a+b) + \frac{c^2-3c}{2} - 14.
 \end{aligned}$$

Since  $n+2-a-b+4-3=0$ , then  $a+b=n+3$ . And so

$$\begin{aligned}
 b_4(G) - b_4(G_n^1) &\geq \frac{(n+3)^2}{2} - \frac{5}{2}(n+3) + \frac{c^2-3c}{2} - 14 - (4n-24) \\
 &= \frac{1}{2}n^2 - \frac{7}{2}n + 7 > 0,
 \end{aligned}$$

and therefore  $b_4(G) > b_4(G_n^1)$ .

If  $l \geq 2$ , by Lemma 1.2,

$$\begin{aligned} b_4(G) &= m(G, 2) - 2s \geq m(G, 2) - 12 \\ &= \frac{(a+b-4)(a+b-7)}{2} + \frac{c(c-3)}{2} + 2(a+b-4-2) \\ &\quad + 2(a+b-4-2) + (c-4)(a+b-4) - 12 \\ &= \frac{(a+b)^2}{2} - \frac{11}{2}(a+b) + (a+b)c + \frac{c^2-11c}{2} - 6. \end{aligned}$$

Since  $n+2-a-b+4-c=0$ , we have  $a+b=n+6-c$ . And so

$$\begin{aligned} b_4(G) - b_4(G_n^1) &\geq \frac{(n+6-c)^2}{2} + (n+6-c)(c-\frac{11}{2}) + \frac{c^2-11c}{2} - 6 - (4n-24) \\ &= \frac{1}{2}n^2 - \frac{7}{2}n + 3, \end{aligned}$$

and hence  $b_4(G) > b_4(G_n^1)$  for  $n \geq 7$ .

When  $t \geq 3$ . Let  $c = t + l$ , then  $c = t + l$ . By Lemma 1.2,

$$\begin{aligned} b_4(G) &= m(G, 2) - 2s \geq m(G, 2) - 12 \\ &= \frac{(a+b-2t)(a+b-2t-3)}{2} + \frac{c(c-3)}{2} + 2(a-t+b-t-2) \\ &\quad + (t-2)(a-t+b-t) + 2(a+b-2t-2) + (l-2)(a+b-2t) - 12 \\ &= \frac{(a+b)^2}{2} - (t+\frac{3}{2})(a+b) + (a+b)l + \frac{c^2-3c}{2} + 3t - 2tl - 20. \end{aligned}$$

Since  $n+2-a-b+2t-c=0$ ,  $c = t + l$ , thus we have  $a+b = n+2+t-l$ . And so

$$\begin{aligned} b_4(G) - b_4(G_n^1) &\geq \frac{(n+2+t-l)^2}{2} - (t+\frac{3}{2})(n+2+t-l) + (n+2+t-l)l \\ &\quad + \frac{c^2-3c}{2} + 3t - 2tl - 20 - (4n-24) \\ &= \frac{n^2}{2} - \frac{7}{2}n + 3, \end{aligned}$$

and hence  $b_4(G) > b_4(G_n^1)$  for  $n \geq 7$ .

Suppose it is true for all graphs  $G \in \mathcal{G}_n$  having exactly six cycles and  $G \not\cong G_n^0, G_n^1, S_n$  with  $n+2-a-b+2t-c < p$  ( $p \geq 1$ ), and suppose  $n+2-a-b+2t-c = p$ , then  $G$  must have pendent edge, say  $uv$ , with pendent vertex  $v$ . By Lemma 1.1,

$$b_4(G) = b_4(G-v) + b_2(G-u-v), \quad b_4(G_n^1) = b_4(G_{n-1}^1) + b_2(K_{1,4}).$$

Notice that  $G-v$  has exactly six cycles on  $n-1$  vertices and  $G \not\cong G_n^0, G_n^1, S_n$ , therefore  $G-v \not\cong G_{n-1}^0, G_{n-1}^1, R_{n-1}, W_{n-1}, Q_{n-1}, S_{n-1}$ , by induction hypothesis,  $b_4(G-v) > b_4(G_{n-1}^1)$ . It is easy to see  $G \not\cong G_n^0, G_n^1, W_n, S_n, Q_n, R_n$ , we have  $b_2(G-u-v) \geq b_2(K_{1,4}) = 4$ . It is immediate that  $b_4(G) > b_4(G_n^1)$  with  $G \not\cong G_n^0, G_n^1, S_n$ .

*Case 2.* There are two cycles contained in  $G$  having exactly one vertex in common. Then choose three cycles, say  $C_a, C_b, C_c$ , such that  $C_a, C_b$  have exactly one vertex in common and the number of edges in  $C_c \setminus (C_a \cup C_b)$  is  $l$ . Then  $n+2-(a+b+l) \geq 0$ , by induction on  $n+2-(a+b+l)$ . If  $n+2-(a+b+l) = 0$ , then by Lemma 1.2,

$$\begin{aligned} b_4(G) &= m(G, 2) - 2s \geq m(G, 2) - 12 \\ &= \frac{a(a-3)}{2} + \frac{b(b-3)}{2} + \frac{(l-1)(l-2)}{2} + (a-2)b + 2(b-2) \\ &\quad + (l-2)(a+b) + 2(a+b-2) - 12 \\ &= \frac{(a+b)^2}{2} - \frac{3}{2}(a+b) + l(a+b) + \frac{l^2-3l}{2} - 19. \end{aligned}$$

Since  $n+2-a-b-l=0$ , so  $a+b=n+2-l$ . And so

$$\begin{aligned} b_4(G) - b_4(G_n^1) &\geq \frac{(n+2-l)^2}{2} - \frac{3}{2}(n+2-l) + l(n+2-l) + \frac{l^2-3l}{2} - 9 - (4n-24) \\ &= \frac{n^2}{2} - \frac{7}{2}n + 4, \end{aligned}$$

thus  $b_4(G) > b_4(G_n^1)$  is immediate for  $n \geq 7$ .

Suppose it is true for all graphs  $G \in \mathcal{G}_n$  having exactly six cycles and  $G \not\cong G_n^0, G_n^1, S_n$  with  $n+2-a-b-l < p$  ( $p \geq 1$ ), and suppose  $n+2-a-b-l = p$ , then  $G$  must have a pendent edge, say  $uv$ , with pendent vertex  $v$ . By Lemma 1.1, we have

$$b_4(G) = b_4(G-v) + b_2(G-u-v), \quad b_4(G_n^1) = b_4(G_{n-1}^1) + b_2(K_{1,4}).$$

Note that  $G-v$  has exactly six cycles on  $n-1$  vertices and  $G \not\cong G_n^0, G_n^1, S_n$ , therefore  $G-v \not\cong G_{n-1}^0, G_{n-1}^1, R_{n-1}, W_{n-1}, Q_{n-1}, S_{n-1}$ , by induction hypothesis,  $b_4(G-v) > b_4(G_{n-1}^1)$ . It is easy to see  $G \not\cong G_n^0, G_n^1, W_n, S_n, Q_n, R_n$ , we have  $b_2(G-u-v) \geq b_2(K_{1,4}) = 4$ . It is immediate that  $b_4(G) > b_4(G_n^1)$  with  $G \not\cong G_n^0, G_n^1, S_n$ .

*Case 3.* There are two cycles contained in  $G$  having no vertex in common. Then choose three cycles, say  $C_a, C_b, C_c$ , such that  $C_a, C_b$  have  $t$  edges in common and  $C_c, C_b$  have  $l$

edges in common. Then  $n+2-(a+b+c)+t+l \geq 0$ , by induction on  $n+2-(a+b+c)+t+l$ . If  $n+2-(a+b+c)+t+l=0$ , i.e.,  $a+b+c=n+2+t+1$ , then by Lemma 1.2,

$$\begin{aligned} b_4(G) &= m(G, 2) - 2s \geq m(G, 2) - 12 \\ &= \frac{(a+b+c-2t-2l)(a+b+c-2t-2l-3)}{2} + \frac{(t-1)(t-2)}{2} \\ &\quad + (t-2)(n+2-t) + 2(n+2-t-2) + \frac{(l-1)(l-2)}{2} \\ &\quad + (l-2)(n+2-t-l) + 2(n+2-t-l-2). \end{aligned}$$

Since  $n+2-(a+b+c)+t+l=0$ , so  $a+b+c=n+2+t+l$ . And so

$$\begin{aligned} b_4(G) - b_4(G_n^1) &\geq \frac{(n+2+t+l-2t-2l)(n+2+t+l-2t-2l-3)}{2} \\ &\quad + \frac{(t-1)(t-2)}{2} + (t-2)(n+2-t) + 2(n+2-t-2) - (4n-24) \\ &\quad + (l-2)(n+2-t-l) + 2(n+2-t-l-2) + \frac{(l-1)(l-2)}{2} \\ &= \frac{n^2}{2} - \frac{7}{2}n + 17 > 0, \end{aligned}$$

thus  $b_4(G) > b_4(G_n^1)$  is immediate.

Suppose it is true for all graphs  $G \in \mathcal{G}_n$  having exactly six cycles and  $G \not\cong G_n^0, G_n^1, S_n$  with  $n+2-a-b-l < p$  ( $p \geq 1$ ), and suppose  $n+2-a-b-l=p$ , then  $G$  must have a pendent edge, say  $uv$ , with pendent vertex  $v$ . By Lemma 1.1, we have

$$b_4(G) = b_4(G-v) + b_2(G-uv), \quad b_4(G_n^1) = b_4(G_{n-1}^1) + b_2(K_{1,4}).$$

Note that  $G-v$  has exactly six cycles on  $n-1$  vertices and  $G \not\cong G_n^0, G_n^1, S_n$ , therefore  $G-v \not\cong G_{n-1}^0, G_{n-1}^1, R_{n-1}, W_{n-1}, Q_{n-1}, S_{n-1}$ , by induction hypothesis,  $b_4(G-v) > b_4(G_{n-1}^1)$ . It is easy to see  $G \not\cong G_n^0, G_n^1, W_n, S_n, Q_n, R_n$ , we have  $b_2(G-uv) \geq b_2(K_{1,4}) = 4$ . It is immediate that  $b_4(G) > b_4(G_n^1)$  with  $G \not\cong G_n^0, G_n^1, S_n$ .

Combining with Cases 1, 2 and 3, this lemma follows.  $\square$

**Lemma 2.5.** *If  $G \in \mathcal{G}_n$  has exactly seven cycles and  $G \not\cong Q_n$ , then  $b_4(G) > b_4(G_n^1)$  for  $n \geq 7$ .*

*Proof.* The configuration of the seven cycles contained in  $G$  is as in Figure 6. Choose

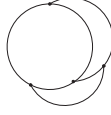


Figure 6: One possible case for the arrangement of seven cycles in  $G$

three cycles, say  $C_a$ ,  $C_b$  and  $C_c$ , such that  $C_a$ ,  $C_b$  have exactly  $t$  edges in common, but all of  $t$  edges are not contained in  $C_c$ . Denote the number of edges of  $C_c$  not contained in  $C_a$  and  $C_b$  by  $l$ . Then  $n + 2 - (a + b - t + l) \geq 0$ . By induction on  $n + 2 - (a + b - t + l)$ . If  $n + 2 - (a + b - t + l) = 0$ .

When  $t = 1$ , by Lemma 1.2

$$\begin{aligned}
 b_4(G) &= m(G, 2) - 2s \geq m(G, 2) - 14 \\
 &= \frac{(a+b-2)(a+b-2-3)}{2} + (a-1+b-1-4+l) + \frac{(l-1)(l-2)}{2} \\
 &\quad + (l-2)(a+b-2) + 2(a+b-2-2) - 14 \\
 &= \frac{(a+b)^2}{2} - \frac{5}{2}(a+b) + \frac{l^2-5l}{2} + l(a+b) - 18.
 \end{aligned}$$

Since  $n + 2 - a - b + 1 - l = 0$ , we have  $a + b = n + 3 - l$ . And so

$$\begin{aligned}
 b_4(G) - b_4(G_n^1) &\geq \frac{(n+3-l)^2}{2} - \frac{5}{2}(n+3-l) + \frac{l^2-5l}{2} + l(n+3-l) \\
 &\quad - 18 - (4n-24) \\
 &= \frac{n^2}{2} - \frac{7}{2}n + 3,
 \end{aligned}$$

it follows that  $b_4(G) > b_4(G_n^1)$  for  $n \geq 7$ .

When  $t = 2$ , by Lemma 1.2

$$\begin{aligned}
 b_4(G) &= m(G, 2) - 2s \geq m(G, 2) - 14 \\
 &= \frac{(a+b-4)(a+b-4-3)}{2} + \frac{(l-1)(l-2)}{2} + 2(a-2+b-2-2+l) \\
 &\quad + (l-2)(a-2+b-2) + 2(a-2+b-2-2) - 14 \\
 &= \frac{(a+b)^2}{2} - \frac{7}{2}(a+b) + l(a+b) + \frac{l^2-7l}{2} - 15.
 \end{aligned}$$



Since  $n + 2 - (a + b - 2 + l) = 0$ , we have  $a + b = n + 4 - l$ . Thus

$$\begin{aligned} b_4(G) - b_4(G_n^1) &\geq \frac{(n+4-l)^2}{2} - \frac{7}{2}(n+4-l) + l(n+4-l) \\ &\quad + \frac{l^2 - 7l}{2} - 15 - (4n - 24) \\ &= \frac{n^2}{2} - \frac{7}{2}n + 3, \end{aligned}$$

and hence  $b_4(G) > b_4(G_n^1)$  for  $n \geq 7$ .

When  $t > 2, l = 1$ , by Lemma 1.2,

$$\begin{aligned} b_4(G) &= m(G, 2) - 2s \geq m(G, 2) - 14 \\ &= \frac{(a+b-2t)(a+b-2t-3)}{2} + \frac{(t-1)(t-2)}{2} + 2(a-t+b-t-2+1) \\ &\quad + (t-2)(a-t+b-t+1) + (a-t+b-t-4) - 14 \\ &= \frac{(a+b)^2}{2} - (t + \frac{1}{2})(a+b) + \frac{t^2+t}{2} - 21. \end{aligned}$$

Since  $n + 2 - (a - t + b + 1) = 0$ , we have  $a + b = n + 1 + t$ . And so

$$\begin{aligned} b_4(G) - b_4(G_n^1) &\geq \frac{(n+1+t)^2}{2} - (t + \frac{1}{2})(n+1+t) + \frac{t^2+t}{2} - 21 - (4n - 24) \\ &= \frac{n^2}{2} - \frac{7}{2}n + 3, \end{aligned}$$

and hence  $b_4(G) > b_4(G_n^1)$  for  $n \geq 7$ .

When  $t > 2, l \geq 2$ , by Lemma 1.2,

$$\begin{aligned} b_4(G) &= m(G, 2) - 2s \geq m(G, 2) - 14 \\ &= \frac{(a+b-2t)(a+b-2t-3)}{2} + \frac{(t-1)(t-2)}{2} + \frac{(l-1)(l-2)}{2} \\ &\quad + 2(a-t+b-t-2) + (t-2)(a-t+b-t+l) + (l-2)(a-t+b-t) \\ &\quad + 2(a-t+b-t-2+l) - 14 \\ &= \frac{(a+b)^2}{2} - (t + \frac{3}{2})(a+b) + l(a+b) + \frac{l^2-3l}{2} + \frac{t^2+3t}{2} - tl - 6. \end{aligned}$$

Since  $n + 2 - (a + b - t + l) = 0$ , we have  $a + b = n + t + 2 - l$ . And so

$$\begin{aligned} b_4(G) - b_4(G_n^1) &\geq \frac{(n+t+2-l)^2}{2} - (t + \frac{3}{2})(n+t+2-l) + l(n+t+2-l) \\ &\quad + \frac{l^2-3l}{2} + \frac{t^2+3t}{2} - tl - 6 - (4n - 24) \\ &= \frac{n^2}{2} - \frac{7}{2}n + 17 > 0. \end{aligned}$$

Namely that  $b_4(G) > b_4(G_n^1)$ .

Suppose it is true for all graphs  $G \in \mathcal{G}_n$  having exactly seven cycles and  $G \not\cong Q_n$  with  $n + 2 - (a + b - t + l) < p$  ( $p \geq 1$ ), and suppose  $n + 2 - (a + b - t + l) = p$ , then  $G$  must have a pendent edge, say  $uv$ , with pendent vertex  $v$ . By Lemma 1.1, we have

$$b_4(G) = b_4(G - v) + b_2(G - u - v), \quad b_4(G_n^1) = b_4(G_{n-1}^1) + b_2(K_{1,4}).$$

Notice that  $G - v$  has exactly seven cycles on  $n - 1$  vertices and  $G \not\cong Q_n$ , therefore  $G - v \not\cong G_{n-1}^0, G_{n-1}^1, W_{n-1}, S_{n-1}, R_{n-1}, Q_{n-1}$ , by induction hypothesis,  $b_4(G - v) > b_4(G_{n-1}^1)$ . It is easy to see  $G \not\cong G_n^0, G_n^1, W_n, S_n, Q_n, R_n$ , we have  $b_2(G - u - v) \geq b_2(K_{1,4}) = 4$ . It is immediate that  $b_4(G) > b_4(G_n^1)$  with  $G \not\cong Q_n$ .  $\square$

By Lemmas 2.2-2.5, we obtain the following proposition.

**Proposition 2.6.** *If  $G \in \mathcal{G}_n$  and  $G \not\cong G_n^0, G_n^1, R_n, W_n, S_n, Q_n$ , then  $E(G) > E(G_n^1)$  for  $n \geq 7$ .*

*Proof.* By Sachs theorem,  $b_0(G) = b_0(G_n^1) = 1$ ,  $b_1(G) = b_1(G_n^1) = 0$ ,  $b_2(G) = b_2(G_n^1) = n + 2$ ,  $b_3(G_n^1) = 0$ ,  $b_i(G_n^1) = 0$  for  $i \geq 5$ . By Lemmas 2.2-2.5,  $b_4(G) > b_4(G_n^1)$  for  $n \geq 7$ . By Lemma 2.1,  $b_{2i}(G) \geq 0$  for  $0 \leq i \leq \lfloor n/2 \rfloor$ . Hence by Coulson integral formula (1.1)

$$E(G) = \frac{1}{\pi} \int_0^{+\infty} \frac{dx}{x^2} \ln \left[ \left( \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} b_{2i}(G)x^{2i} \right)^2 + \left( \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} b_{2i+1}(G)x^{2i+1} \right)^2 \right],$$

$$E(G_n^1) = \frac{1}{\pi} \int_0^{+\infty} \frac{dx}{x^2} \ln \left[ \left( \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} b_{2i}(G_n^1)x^{2i} \right)^2 \right].$$

From these formulas it is immediate to show that  $E(G) > E(G_n^1)$ .  $\square$

**Proposition 2.7.** (i)  $E(G_n^0) < E(G_n^1)$  for  $n \geq 11$ .

(ii)  $E(G_n^1) < E(G_n^0), E(R_n), E(W_n), E(S_n), E(Q_n)$  for  $7 \leq n \leq 10$ .

*Proof.* (i) We want to determine the characteristic polynomial of  $G_n^0$  (respectively,  $G_n^1$ ). In fact, by Sachs theorem we can obtain  $a_0 = 1, a_1 = 0, a_2 = -(n + 2), a_3 = -6, a_4 = 3n - 15$  and  $a_i = 0$  for  $i \geq 5$ . It follows that

$$\phi(G_n^0, \lambda) = \lambda^n - (n + 2)\lambda^{n-2} - 6\lambda^{n-3} + (3n - 15)\lambda^{n-4}.$$

Similarly, for  $G_n^1$ , we obtain  $a'_0 = 1, a'_1 = 0, a'_2 = -(n+2), a'_3 = 0, a'_4 = 4n-24$  and  $a'_i = 0$  for  $i \geq 5$ , and so

$$\phi(G_n^1, \lambda) = \lambda^n - (n+2)\lambda^{n-2} + (4n-24)\lambda^{n-4}.$$

By (1.1),

$$E(G_n^1) - E(G_n^0) = \frac{1}{\pi} \int_0^\infty \frac{dx}{x^2} \ln \frac{[1 + (n+2)x^2 + (4n-24)x^4]^2}{[1 + (n+2)x^2 + (3n-15)x^4]^2 + 36x^6}.$$

Let

$$\begin{aligned} f(x) &= [1 + (n+2)x^2 + (4n-24)x^4]^2 - [1 + (n+2)x^2 + (3n-15)x^4]^2 - 36x^6 \\ &= 2(n-9)x^4 + (n-9)(7n-39)x^8 + 2 \left[ \left( n - \frac{7}{2} \right)^2 - \frac{193}{4} \right] x^6. \end{aligned}$$

It follows that  $f(x) > 0$  for  $n \geq 11$ . Hence  $E(G_n^0) < E(G_n^1)$  for  $n \geq 11$ .

(ii) By direct calculation (rounded to four decimal places), we have

$$\begin{array}{llll} E(G_7^0) = 7.5238, & E(G_8^0) = 8.0455, & E(G_9^0) = 8.5019, & E(G_{10}^0) = 8.9134, \\ E(G_7^1) = 6.0000, & E(G_8^1) = 6.3246, & E(G_9^1) = 6.6332, & E(G_{10}^1) = 6.9282, \\ E(R_7) = 10.0000, & E(R_8) = 10.5461, & E(R_9) = 11.0158, & E(R_{10}) = 11.4354, \\ E(W_7) = 8.8703, & E(W_8) = 9.4027, & E(W_9) = 9.8647, & E(W_{10}) = 10.2795, \\ E(S_7) = 6.2548, & E(S_8) = 6.8284, & E(S_9) = 7.2524, & E(S_{10}) = 7.6402, \\ E(Q_7) = 8.2653, & E(Q_8) = 8.7446, & E(Q_9) = 9.1638, & E(Q_{10}) = 9.5662. \end{array}$$

It is immediate that the results hold. □

Unfortunately, using above method, we can not compare the values of  $E(G)$  with  $E(G_n^0)$  for  $G \in \mathcal{G}_n$  and  $G \not\cong R_n, S_n, W_n, Q_n, G_n^0$ . Hence, combining Propositions 2.6 and 2.7, we obtain the following main results of this paper.

**Theorem 2.8.** (i)  $G_n^1$  has minimal energy in  $\mathcal{G}_n$  for  $7 \leq n \leq 10$ .

(ii) If  $G \in \mathcal{G}_n$  and  $G \not\cong R_n, W_n, S_n, Q_n, G_n^0, G_n^1$ , then  $E(G_n^0) < E(G_n^1) < E(G)$  for  $n \geq 11$ .

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