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On tetracyclic 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 $\mathscr{G}_n$ be the class of tetracyclic 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 value on the energies of the graphs in $\mathscr{G}_n$ and determine the corresponding graphs.

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

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

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

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

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 $\lambda_1, \ldots, \lambda_n$ 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 π-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 $E(G)$ can be expressed as the Coulson integral formula [12]

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

Let $b_{2i}(G) = (-1)^i a_{2i}$ and $b_{2i+1}(G) = (-1)^i a_{2i+1}$ for $0 \leqslant i \leqslant \lfloor \frac{n}{2} \rfloor$. 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 $b_i(G), i = 1, \ldots, \lfloor n/2 \rfloor$.

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 $n \geqslant 6$ vertices, $n-1 \leqslant e \leqslant 2(n-2)$ edges and minimum energy are star with $e-n+1$ additional edges all connected to the same vertex for $e \leqslant n + \lfloor \frac{n-7}{2} \rfloor$, 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 $e = n$ for $n \geqslant 6$ [17]. When $e = n+1$ and $e = n+2$ the conjecture has been discussed [40, 26]. In this paper, we consider the above conjecture for the case $e = n+3$ for $n \geqslant 9$.

G_n^0 G_n^1

Figure 1: Graphs G_n^0 and G_n^1

A connected simple graph with n vertices and $e = n + 3$ edges contains four elementary cycles and called *tetracyclic*. Let $\mathscr{G}_n$ be the class of tetracyclic graphs 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 4 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 $n - 5$ pendent vertices to a vertex of degree 5 of the complete bipartite graph $K_{2,5}$ (e.g., see Figure 1). In this paper, for graphs in $\mathscr{G}_n$, we show that G_n^0 has minimal energy if $n \geqslant 18$ and G_n^1 has the minimal energy if $9 \leqslant n \leqslant 17$.

The following two lemmas are needed in our paper.

Lemma 1.2 ([40]). *Let G be a graph with n vertices and let uv be a pendent edge of G with pendent vertex v. Then for $2 \leqslant i \leqslant n$, $b_i(G) = b_i(G - v) + b_{i-2}(G - u - v)$.*

Lemma 1.3 ([40]). *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 graphs in $\mathscr{G}_n$ $(n \geqslant 9)$ having the minimal energy.

We are, at first, to show $E(G) > E(G_n^1)$ for any $G \in \mathscr{G}_n$ with $G \notin \mathscr{J}_n$; and proceed to show that $E(G_n^0) < E(G_n^1)(n \geq 18)$, and $E(G_n^1) < E(G_n^0)(9 \leq n \leq 17)$, where each graph in $\mathscr{J}_n$ is as shown in Figure 2. The following fact is immediate.

Fact 1. *For any $G \in \mathscr{G}_n$, there are at most four vertex-disjoint cycles contained in G.*

Lemma 2.1. *If $G \in \mathscr{G}_n$, then $b_{2i} \geqslant 0$ for $0 \leqslant i \leqslant \lfloor \frac{n}{2} \rfloor$.*

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 $b_{2i}(G) = \sum_{S \in L_{2i}} 1 \geqslant 0$. Otherwise, there exists S' in L_{2i} such that S' contains cycles. If S' has no odd cycles, then $b_{2i}(G) \geqslant 0$ [14]; If S' contains odd cycles, together with Fact 1, S' must contain two or four vertex-disjoint odd cycles.

Case 1. If S' contains two odd cycles, say C_k, C_l, we have $k+l \equiv 0 \pmod 4$ since $G \in \mathscr{G}_n$. 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' contains one more cycle C_m besides C_k, C_l, then C_m must be even. Thus its corresponding term in b_{2i} is $(-1)^{p(S')+i} 2^3$. 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. Their corresponding terms in b_{2i} are

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

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 $|L_{2i}^1| \geqslant 2|L_{2i}^2|$, and so

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

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

Case 2. If S' contains four odd cycles, say $C_{l_i}(i = 1, 2, 3, 4)$, then C_{l_i} must be pairwise vertex-disjoint. We have $l_p + l_q \equiv 0 \pmod 4$ $(p, q = 1, 2, 3, 4, p \neq q)$. Note that S' has no five pairwise vertex-disjoint cycles. Then

$$p(S') + i = 4 + \frac{2i - (l_1 + l_2 + l_3 + l_4)}{2} + i \equiv 0 \pmod 2.$$

Hence $b_{2i} \geq 0$. $\square$

In $\mathscr{G}_n$, there exist eight special graphs, $G_i(i = 1, \cdots, 8)$; see Figure 2, where G_1 (G_2) has $n - 9$ ($n - 8$, *repectively*) pendent vertices, each of G_3 and G_4 has $n - 7$ pendent vertices, each of G_5 and G_6 has $n - 6$ pendent vertices, and each of G_7 and G_8 has $n - 5$ pendent vertices.

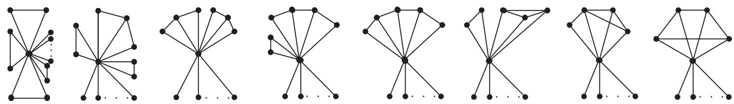

Figure 2: Graphs $G_1, G_2, G_3, G_4, G_5, G_6, G_7$ and G_8.

Let $\mathscr{J}_n = \{G_n^0, G_n^1, G_1, G_2, G_3, G_4, G_5, G_6, G_7, G_8\}$ (see Figure 1 and Figure 2). It is straightforward to check that graph $G \in \mathscr{G}_n$ has at least 4 cycles and at most 15 cycles but has no 9 cycles.

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 $G \in \mathscr{G}_n$ and $G \notin \mathscr{J}_n$, then $b_4(G) > b_4(G_n^1)$ for $n \geqslant 9$.*

Proof. First we assume that G contains pendent edges, let uv be a pendent edge of G with pendent vertex v. By Lemma 1.2,

$$b_4(G) = b_4(G - v) + b_2(G - u - v), \quad b_4(G_n^1) = b_4(G_{n-1}^1) + b_2(K_{1,5}).$$

Note that $G - v$ has exactly four cycles on $n - 1$ vertices and $G \notin \mathscr{J}_n$, therefore $G - v \notin \mathscr{J}_{n-1}$, by induction hypothesis, $b_4(G - v) > b_4(G_{n-1}^1)$. It is easy to see $G - u - v \notin \mathscr{J}_{n-2}$, we have $b_2(G - u - v) \geqslant b_2(K_{1,5}) = 5$. It is immediate that $b_4(G) > b_4(G_n^1)$.

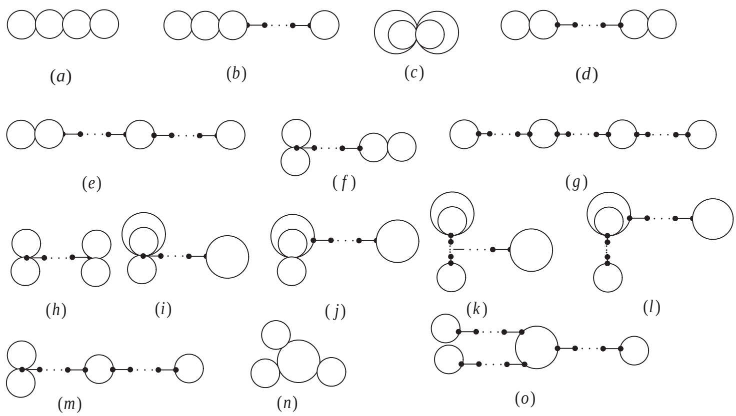

Figure 3: 15 possible cases for the arrangement of four cycles in G.

Second we assume that G contains no pendent edges. Please note that G has at least 4 cycles and at most 15 cycles. So we consider the following several cases.

Case 1. G contains exactly four cycles.

Without loss of generality, let four cycles be C_a, C_b, C_c and C_d. These four cycles must be edge-disjoint; see Figure 3.

Note that any two adjacent edges cannot be a 2-match.

Subcase 1-1 Graphs (a), (b), (d) and (g) in Figure 3.

For the graph G being (g) in Figure 3, assume that there is a path P_{i_j} connecting C_i and C_j and by Lemma 1.3,

$$\begin{aligned} b_4(G) &= m(G,2) - 2s \geqslant m(G,2) - 8 \\ &= \frac{(n+3)(n+2)}{2} - (\sum |C_i| + \sum_{i_j} \max(|P_{i_j}| - 1, 0)) - 12 - 8 \\ &\geqslant \frac{n^2+5n+6}{2} - (n+3) - 20 = \frac{n^2}{2} + \frac{3n}{2} - 20. \\ b_4(G) - b_4(G_n^1) &\geqslant \frac{1}{2}n^2 + \frac{1}{2}n - 18 - (5n-35) = \frac{1}{2}n^2 - \frac{7}{2}n + 15 > 0. \end{aligned}$$

Graph (a)(graph (b),(d) and (e), respectively) is a special case of graph (g) with $|P_{i_j}| = 0$ ($|P_{c_d}| = 0, |P_{b_c}| = 0$ and $|P_{b_c}| = |P_{c_d}| = 0$, respectively). To avoid repetition, we omit the proof here.

Subcase 1-2 Graphs (c) and (h).

For the graph G being (h) in Figure 3, assume that there is a path P_k

connecting C_a, C_b and C_c, C_d and by Lemma 1.3,

$$\begin{aligned}
b_4(G) &\geqslant m(G,2) - 8 = \frac{(n+3)(n+2)}{2} \\
&\quad -(\sum(|C_i|) + \max(|P_k| - 1, 0)) - 16 - 8 \\
&\geqslant \frac{n^2+5n+6}{2} - (n+3) - 24 = \frac{n^2}{2} + \frac{3n}{2} - 24. \\
b_4(G) - b_4(G_n^1) &\geqslant \frac{1}{2}n^2 + \frac{3}{2}n - 24 - (5n-35) = \frac{1}{2}n^2 - \frac{7}{2}n + 11 > 0.
\end{aligned}$$

Graph (c) is a special case of graph (h) with $|P_k| = 0$, to avoid repetition, we omit the proof here.

Subcase 1-3 Graphs (i), (j), (k) and (l).

For the graph G being (l) in Figure 3, assume that there is a path P_k connecting C_a and C_d, another path P_r connecting $C_a(C_b)$ and C_c. We have

$$\begin{aligned}
b_4(G) &\geqslant \frac{(n+3)(n+2)}{2} \\
&\quad -(\sum(|C_i|) + \max(|P_k| - 1, 0) + \max(|P_r| - 1, 0)) - 14 - 8 \\
&\geqslant \frac{n^2+5n+6}{2} - (n+3) - 22 = \frac{n^2}{2} + \frac{3n}{2} - 22. \\
b_4(G) - b_4(G_n^1) &\geqslant \frac{1}{2}n^2 + \frac{3}{2}n - 22 - (5n-35) = \frac{1}{2}n^2 - \frac{7}{2}n + 13 > 0.
\end{aligned}$$

Discussion for the value of b_4 of Graph (i),(j) and (k) is similar to that of graph (l) and b_4 is no less than the value of b_4 of graph (l), so we omit the proof here.

Subcase 1-4 Graphs (f) and (m).

For the graph G being (m) in Figure 3, assume that there is a path P_k connecting C_a, C_b and C_c, another path P_r connecting C_c and C_d. We have

$$\begin{aligned}
b_4(G) &\geqslant \frac{(n+3)(n+2)}{2} \\
&\quad -(\sum(|C_i|) + \max(|P_k| - 1, 0) + \max(|P_r| - 1, 0)) - 14 - 8 \\
&\geqslant \frac{n^2+5n+6}{2} - (n+3) - 22 = \frac{n^2}{2} + \frac{3n}{2} - 22. \\
b_4(G) - b_4(G_n^1) &\geqslant \frac{1}{2}n^2 + \frac{3}{2}n - 22 - (5n-35) = \frac{1}{2}n^2 - \frac{7}{2}n + 13 > 0.
\end{aligned}$$

Graph (f) is a special case of graph (m) with $|P_r| = 0$, so we omit its proof.

Subcase 1-5 Graphs (n) and (o).

For the graph G being (o) in Figure 3, assume that there is a path P_{a_i} connecting C_a and $C_i (i = b, c, d)$. We have

$$\begin{aligned} b_4(G) &\geqslant \frac{(n+3)(n+2)}{2} - (\sum |C_i| + \max(|P_{a_i}| - 1, 0)) - 12 - 8 \\ &\geqslant \frac{n^2+5n+6}{2} - (n+3) - 22 = \frac{n^2}{2} + \frac{3n}{2} - 22 \\ b_4(G) - b_4(G_n^1) &\geqslant \frac{1}{2}n^2 + \frac{3}{2}n - 22 - (5n - 35) = \frac{1}{2}n^2 - \frac{7}{2}n + 13 > 0. \end{aligned}$$

Graph (n) is a special case of graph (o) with $|P_{a_i}| = 0$, so we omit its proof.

Hence, we complete discussion of case 1.

Case 2. $G \in \mathscr{G}_n$ with $G \notin \mathscr{J}_n$ has exactly five cycles. Since G has exactly five cycles, by Fact 1, there are exactly two cycles, say C_a and C_b, having t $(t \geqslant 1)$ common edges and each of C_a, C_b has no common edges with each of rest two cycles C_c, C_d, and C_c and C_d are edge-disjoint (see graphs in Figure 4).

Subcase 2-1 Graphs (a), (i) and (f).

We consider graph (i) in Figure 4 first.

Note that any two adjacent edges cannot be a 2-match. For the graph G being (i) in Figure 4, where P_k connects C_a and $C_c(C_d)$, we have

$$\begin{aligned} b_4(G) &\geqslant \frac{(n+3)(n+2)}{2} \\ &\quad -((\sum |C_i|) - t + \max(|P_k| - 1, 0))) - 14 - 10 \\ &= \frac{(n^2+5n+6)}{2} - (n+3) - 24 = \frac{1}{2}n^2 + \frac{3}{2}n - 24. \\ b_4(G) - b_4(G_n^1) &= \frac{1}{2}n^2 - \frac{7}{2}n + 11 > 0. \end{aligned}$$

Graph (a) (graph (f), respectively) is a special case of graph (i) with $|P_k| = 0$ (P_k share a common vertex with both C_a and C_b, respectively).

Subcase 2-2 Graphs (c),(d), (e) and (j).

For the graph G being (d) in Figure 4, where P_k connects $C_a(C_b)$ and C_c, and P_r connects C_c and C_d, we have

$$\begin{aligned} b_4(G) &\geqslant \frac{(n+3)(n+2)}{2} - ((\sum |C_i|) - t + \max(|P_k| - 1, 0)) + \\ &\quad \max(|P_r| - 1, 0)) - 13 - 10 \\ &\geqslant \frac{(n^2+5n+6)}{2} - (n+3) - 23 = \frac{1}{2}n^2 + \frac{3}{2}n - 23. \\ b_4(G) - b_4(G_n^1) &= \frac{1}{2}n^2 - \frac{7}{2}n + 12 > 0. \end{aligned}$$

Graph (e) is a special case of graph (d) with $|P_r| = 0$. Discussion of graph (e) is similar to that of graph (d) and graph (j) is a special case of graph (e). So we omit the proof here.

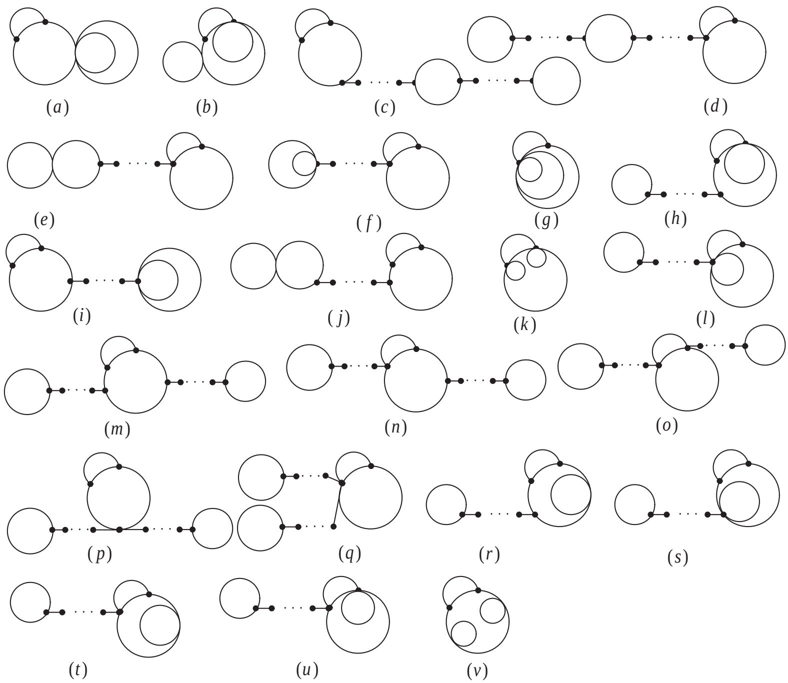

Figure 4: 22 possible cases for the arrangement of five cycles in G

Subcase 2-3 Graphs (b), (h), (k),(m),(n) and (o).

For the graph G being (m) in Figure 4, where P_k connects C_a and C_c, and P_r connects C_a and C_d. we have

$$\begin{aligned} b_4(G) &\geqslant m(G,2)-10 \\ &= \frac{(n+3)(n+2)}{2} - ((\sum |C_i|) - t + \max(|P_k|-1,0)) + \\ &\quad \max(|P_r|-1,0)) - 12 - 10 \\ &\geqslant \frac{(n^2+5n+6)}{2} - (n+3) - 22 = \frac{1}{2}n^2 + \frac{3}{2}n - 22. \\ b_4(G) - b_4(G_n^1) &\geqslant \frac{1}{2}n^2 - \frac{7}{2}n + 13 > 0. \end{aligned}$$

Graph (n) in Figure 4 is a special case of graph (m) with P_k sharing a common vertex with both C_a and C_b. We have $b_4(G)-b_4(G_n^1) \geqslant \frac{1}{2}n^2-\frac{7}{2}n+12 > 0$. Similarly, for graph (o), $b_4(G) - b_4(G_n^1) \geqslant \frac{1}{2}n^2 - \frac{7}{2}n + 11 > 0$. Graph (k) (graph (h) and graph (b), respectively) is a special case of graph (o) (graph (n), respectively) with $|P_k| = |P_r| = 1$ ($|P_r| = 1$ and $|P_k| = |P_r| = 1$, respectively). Hence, we omit the proof here.

Subcase 2-4 Graphs (g), (p), (q) and (s).

For the graph G being (p) in Figure 4, where P_k connects C_a and C_c, and P_r connects C_a and C_d with P_k, P_r sharing an end vertex, we have

$$\begin{aligned} b_4(G) &\geqslant m(G,2) - 10 \\ &= \frac{(n+3)(n+2)}{2} - ((\sum |C_i|) - t + \max(|P_k| - 1, 0)) + \\ &\quad \max(|P_r| - 1, 0)) - 12 - 10 \\ &\geqslant \frac{(n^2+5n+6)}{2} - (n+3) - 22 = \frac{1}{2}n^2 + \frac{3}{2}n - 22. \\ b_4(G) - b_4(G_n^1) &\geqslant \frac{1}{2}n^2 - \frac{7}{2}n + 13 > 0. \end{aligned}$$

Graph (s)(graph (q), respectively) is a special case of graph (p) with $P_r = 1$ (both P_r, P_k sharing a common vertex with $C_a(C_b)$, respectively). Graph (g) is a special case of (q). For each graph G listed above, we have $b_4(G) - b_4(G_n^1) \geqslant \frac{1}{2}n^2 - \frac{7}{2}n + 11 > 0$.

Subcase 2-5 Graphs (r), (u), (v) and (t).

For the graph G being (r) in Figure 4, where P_k connects C_a and C_c, C_d and C_a share a common vertex, we have

$$\begin{aligned} b_4(G) &\geqslant \frac{(n+3)(n+2)}{2} \\ &\quad -((\sum |C_i|) - t + \max(|P_k| - 1, 0)) - 12 - 10 \\ &\geqslant \frac{(n^2+5n+6)}{2} - (n+3) - 22 = \frac{1}{2}n^2 + \frac{3}{2}n - 22. \\ b_4(G) - b_4(G_n^1) &\geqslant \frac{1}{2}n^2 - \frac{7}{2}n + 13 > 0. \end{aligned}$$

Graph (t)(graph (v), respectively) is a special case of graph (r) and graph (u) is a special case of (t). For each graph G listed above, we have $b_4(G) - b_4(G_n^1) \geqslant \frac{1}{2}n^2 - \frac{7}{2}n + 12 > 0$. Since the calculation is similar, it is omitted here. Thus we complete the discussion of case 2.

Case 3. $G \in \mathscr{G}_n$ has exactly six cycles.

All possible graphs with six cycles are listed in Figure 5. Without loss of generality, we consider graph G being (a), (e) and (f) in Figure 5 only. For graph (a), it has two pairs of cycles $\{C_a, C_b\}$ and $\{C_c, C_d\}$ sharing some common edges. Let C_a and C_b share t_1 common edges, C_c and C_d share t_2 edges and there is a path P_k connecting C_b and C_d (see Figure 5 (a)).

Since G has no pendent vertex, then

$$\begin{aligned} b_4(G) &= m(G,2) - 2s \geqslant m(G,2) - 12 \\ &\geq \frac{n^2+5n+6}{2} - (|C_a| + |C_b| + |C_c| + |C_d| - t_1 - t_2 + \\ &\quad \max(|P_k| - 1, 0)) - 12 - 12 \\ &\geq \frac{(n+3)(n+2)}{2} - (n+3) - 12 - 12 = \frac{1}{2}n^2 + \frac{3}{2}n - 24. \end{aligned}$$

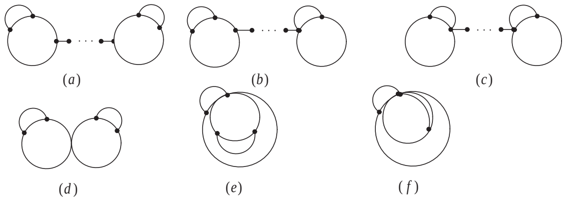

Figure 5: 6 possible cases for the arrangement of six cycles in G

$$b_4(G) - b_4(G_n^1) \;=\; \frac{1}{2}n^2 + \frac{3}{2}n - 24 - (5n - 35) = \frac{n^2}{2} - \frac{7n}{2} + 11 > 0.$$

Graph (d) ((b), (c) respectively) is a special case of (a) with $|P_k| = 1$ (one of end vertices of P_k is a common vertex of C_c and C_d, two end vertices of P_k sharing a common vertex with $C_a(C_b)$ and $C_c(C_d)$, respectively), we omit the discussion here. For graph (e), $b_4(G) - b_4(G_n^1) \geqslant \frac{1}{2}n^2 + \frac{3}{2}n - 26 - (5n - 35) = \frac{n^2}{2} - \frac{7n}{2} + 9 > 0$. For graph (f), we have $b_4(G) - b_4(G_n^1) \geqslant \frac{1}{2}n^2 + \frac{3}{2}n - 28 - (5n - 35) = \frac{n^2}{2} - \frac{7n}{2} + 7 > 0$.

Case 4. $G \in \mathscr{G}_n$ has exactly seven cycles.

Some configurations of graphs G containing seven cycles are exhibited in Figure 6.

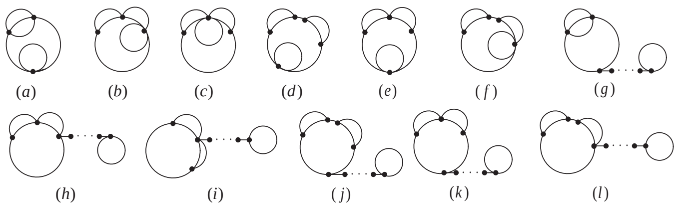

Figure 6: 12 possible arrangements of seven cycles in G

Subcase (4-1) Graphs (a) and (g) in Figure 6.

We consider graph (g) in Figure 6. Let C_a, C_b and C_c have t edges in common. There is a path P_k connecting C_a and C_d.

$$\begin{aligned} b_4(G) &= m(G,2) - 2s \geqslant m(G,2) - 14 \geq \frac{n^2+5n+6}{2} \\ &\quad -(|C_a| + |C_b| + |C_c| + |C_d| - t_1 - t_2 + \max(|P_k| - 1, 0)) - 14 - 14 \\ &= \frac{n^2+5n+6}{2} - (n+3) - 14 - 14 \\ &= \frac{1}{2}n^2 + \frac{3}{2}n - 28. \end{aligned}$$

$$b_4(G) - b_4(G_n^1) \geqslant \frac{1}{2}n^2 + \frac{3}{2}n - 28 - (5n - 35) = \frac{1}{2}n^2 - \frac{7}{2}n + 7 > 0.$$

Clearly graph (a) is a special case of (g) with $|P_k| = 1$.

Subcase (4-2) Graphs (b),(f), (h) and (l) in Figure 6.

We consider a graph (l). Let C_a and C_b have t_1 common edges, C_a and C_c have t common edges in common. P_k connects C_a and C_d with one end vertex joining C_a and C_b.

$$\begin{aligned} b_4(G) &\geq \frac{n^2+5n+6}{2} \\ &\quad -(|C_a| + |C_b| + |C_c| + |C_d| - t_1 - t_2 + \max(|P_k| - 1, 0)) \\ &\quad -13 - 14 \\ &= \frac{n^2+5n+6}{2} - (n+3) - 13 - 14 = \frac{1}{2}n^2 + \frac{3}{2}n - 27. \\ b_4(G) - b_4(G_n^1) &\geqslant \frac{1}{2}n^2 + \frac{3}{2}n - 28 - (5n - 35) = \frac{1}{2}n^2 - \frac{7}{2}n + 8 > 0. \end{aligned}$$

Clearly graph (f) (graph (h) respectively) is a special case of (l) with $|P_k| = 1$ (C_a, C_b and C_c sharing one vertex, respectively). While graph (b) is a special case of (h) with $|P_k| = 1$.

Subcase (4-3) Graphs (c),(d),(e), (k), (i) and (j).

Calculation the value of b_4 for each graph listed in Subcase (4-3) is similar as in Subcase (4-2), so we omit it here. And we have $b_4 - b_4(G_n^1) > 0$.

Case 5. $G \in \mathscr{G}_n$ has exactly eight cycles.

The four configurations of graphs G containing eight cycles exhibited in Figure 7.

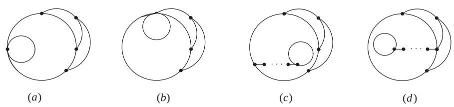

Figure 7: 4 possible arrangements of eight cycles in G

Without loss of generality, we consider a graph G in Figure 7 (c). Let C_a and C_b have t_1 edges in common, C_a and C_c have t_2 edges in common, C_b and C_c have t_3 edges in common. A path P_k connects C_a and C_d.

$$\begin{aligned} b_4(G) &= m(G,2) - 2s \geqslant m(G,2) - 16 \\ &\geq \frac{n^2+5n+6}{2} - (|C_a| + |C_b| + |C_c| + |C_d| - t_1 - t_2 - t_3 \\ &\quad + \max(|P_k| - 1, 0)) - 12 - 16 \\ &= \frac{1}{2}n^2 + \frac{3}{2}n - 28. \\ b_4(G) - b_4(G_n^1) &\geqslant \frac{1}{2}n^2 + \frac{3}{2}n - 28 - (5n - 35) \\ &= \frac{1}{2}n^2 - \frac{7}{2}n + 7 > 0. \end{aligned}$$

Similarly, for graph (d), we have $b_4(G)-b_4(G_n^1)\geqslant \frac{1}{2}n^2+\frac{3}{2}n-28-(5n-35)=\frac{1}{2}n^2-\frac{7}{2}n+6>0$.

Note that graph (a)(graph (b), respectively) is a special case of graph (c)(graph (d), respectively).

Case 6. $G\in\mathscr{G}_n$ contains exactly 11 cycles.

Note that there is no 9-cycle graphs in $\mathscr{G}_n$. Without loss of generality and to avoid the repetition, we are to verify one graph (a) in Figure 8.

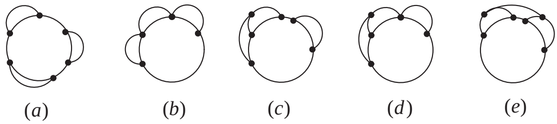

Figure 8: 7 possible cases for the arrangement of 11 cycles in G

Note that there is no pendent edges in G, without loss of generality, we consider the graph G in Figure 8 (a). Let C_i and C_j have $t_{i,j}$ $(i,j=1,2,3,i\neq j)$ edges in common, then

$$\begin{aligned}
b_4(G) &= m(G,2)-2s\geqslant m(G,2)-22\\
&\geq \frac{n^2+5n+6}{2}-(|C_a|+|C_b|+|C_c|+|C_d|-t_{a,b}-t_{a,c}-t_{a,d})-12-22\\
&= \frac{n^2+5n+6}{2}-(n+3)-12-22=\frac{1}{2}n^2+\frac{3}{2}n-34.
\end{aligned}$$

$$b_4(G)-b_4(G_n^1)\ \geqslant\ \frac{1}{2}n^2+\frac{3}{2}n-34-(5n-35)=\frac{1}{2}n^2-\frac{7}{2}n+1>0(n\geq 8).$$

Graph (b) is a special case of (a). We have

$$\begin{aligned}
b_4(G) &= m(G,2)-2s\geqslant m(G,2)-22\\
&\geq \frac{n^2+5n+6}{2}-(|C_a|+|C_b|+|C_c|+|C_d|-t_{a,b}-t_{a,c}-t_{a,d})-13-22\\
&= \frac{n^2+5n+6}{2}-(n+3)-13-22=\frac{1}{2}n^2+\frac{3}{2}n-35.
\end{aligned}$$

$$b_4(G)-b_4(G_n^1)\geq \frac{1}{2}n^2+\frac{3}{2}n-34-(5n-35)=\frac{1}{2}n^2-\frac{7}{2}n>0(n\geq 8).$$

For graph (c) in Figure 8,

$$\begin{aligned}
b_4(G) &= m(G,2)-2s\geqslant m(G,2)-22\\
&\geq \frac{n^2+5n+6}{2}\\
&\quad -(|C_a|+|C_b|+|C_c|+|C_d|-t_{a,b}-t_{a,c}-t_{a,d}-t_{c,d})-12-22\\
&= \frac{1}{2}n^2+\frac{3}{2}n-34.
\end{aligned}$$

$$b_4(G) - b_4(G_n^1) \geqslant \frac{1}{2}n^2 + \frac{3}{2}n - 34 - (5n - 35) = \frac{1}{2}n^2 - \frac{7}{2}n + 1 > 0 (n \geq 8).$$

Graph (d) is a special case with C_b and C_c sharing a common vertex on C_a.

For graph (e), we have

$$b_4(G) \geq \frac{n^2 + 5n + 6}{2} - (\sum(|C_i|) - t_{a,b} - t_{a,c} - t_{a,d} - t_{b,d} - t_(c,d)) - 12 - 22$$

$$b_4(G) - b_4(G_n^1) \geq \frac{1}{2}n^2 + \frac{3}{2}n - 34 - (5n - 35) = \frac{1}{2}n^2 - \frac{7}{2}n + 1 > 0 (n \geq 8).$$

Case 7. $G \in \mathscr{G}_n$ contains exactly i $(i = 10, 12, 13, 14, 15)$ cycles.

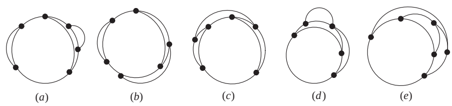

Figure 9: Some possible arrangements of 10,12,13,14 15 cycles in G

For $i = 10, 12, 13, 14$ and 15, we find exactly one graph with exactly i cycles. Let cycle C_i and cycle C_j have $t_{i,j}$ edges in common, where $i = a, b, c, d$, $j = b, c, d (i \neq j)$. Note that the value of $t_{i,j}$ may be zero for some graph. For instance, graph (a) has $t_{a,c} = t_{a,d} = t_{b,d} = 0$.

Note that graph (e) has the least value of b_4. For each i-cycle graph G $(i = 10, 12, 13, 14, 15)$ in Figure 9, we have

$$\begin{aligned} b_4(G) &= m(G,2) - 2s \geqslant \frac{n^2 + 5n + 6}{2} \\ &- (|C_a| + |C_b| + |C_c| + |C_d| - t_{a,b} - t_{a,c} - t_{a,d} - t_{b,c} - t_{b,d} - t_{c,d}) \\ &\quad -12 - 2i \\ &= \frac{n^2 + 5n + 6}{2} - (n + 3) - 12 - 3i = \frac{1}{2}n^2 + \frac{3}{2}n + 12 - 2i \\ b_4(G) - b_4(G_n^1) &\geq \frac{1}{2}n^2 + \frac{3}{2}n - 42 - (5n - 35) = \frac{1}{2}(n - \frac{7}{2})^2 + 23 - 2i \\ &\geqslant \frac{1}{2}(n - \frac{7}{2})^2 - 42 \geqslant \frac{1}{2}(n - \frac{7}{2})^2 - \frac{105}{8} > 0 (n \geq 9). \end{aligned}$$

□

By previous Lemma, we obtain the following proposition.

Proposition 2.3. *If $G \in \mathscr{G}_n$ and $G \notin \mathscr{J}_n$, then $E(G) > E(G_n^1)$ for $n \geqslant 9$.*

Proof. By Sachs theorem, for each graph in $\mathscr{G}_n$, we have $b_0 = 1$, $b_1 = 0$, $b_2 = n+3$, for G_n^1, $b_3(G_n^1) = 0$, $b_4(G_n^1) = 5n-35, b_i(G_n^1) = 0$ for $i \geqslant 5$. By previous Lemma, $b_4(G) > b_4(G_n^1)$ for $n \geqslant 9$. By Lemma 2.1, $b_{2i}(G) \geqslant 0$ for $0 \leqslant i \leqslant \lfloor n/2 \rfloor$. Hence by Coulson integral formula (1.1),

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

From these formulas it is immediate that $E(G) > E(G_n^1)$. □

Lemma 2.4. *For each $G_j \in \mathscr{J}_n (j = 1, \cdots, 8)$ (see Figure 2),*

(i) $E(G_n^0) < E(G_j)$ *for* $n \geqslant 9$.

(ii) $E(G_n^1) < E(G_j)$ *for* $9 \leqslant n \leqslant 17$.

Proof. Note that for each graph $G \in \mathscr{G}_n$, $b_0(G) = 1, b_1(G) = 0, b_2(G) = n+3, b_3(G) = 8$. So we need to find $b_i (i \geq 4)$ for each $G_k (k = 1, \cdots, 8)$ only. For each G_j, we list the $b_i(G_j)$ as below.

$$\begin{array}{llll} b_4(G_1) = 4n-6, & b_4(G_2) = 4n-7, & b_4(G_3) = 4n-8, & b_4(G_4) = 4n-8, \\ b_5(G_1) = 24, & b_5(G_2) = 20, & b_5(G_3) = 16, & b_5(G_4) = 16, \\ b_6(G_1) = 6n-26, & b_6(G_2) = 5n-23, & b_6(G_3) = 4n-20, & b_6(G_4) = 3n-1, \\ b_7(G_1) = 24, & b_7(G_2) = 12, & & b_7(G_4) = 6, \\ b_8(G_1) = 4n-27, & b_8(G_2) = 2n-16, & & \\ b_9(G_1) = 8. & & & \end{array}$$

$$\begin{array}{llll} b_4(G_5) = 4n-9, & b_4(G_6) = 4n-9, & b_4(G_7) = 4n-15, & b_4(G_8) = 4n-16, \\ b_5(G_5) = 12, & b_5(G_6) = 2n-2, & b_5(G_7) = 2n-6, & b_5(G_8) = 8, \\ b_6(G_5) = 3n-15, & b_6(G_6) = 3n-15, & b_6(G_7) = n-5, & b_6(G_8) = 2n-10, \\ & b_7(G_6) = 2n-12, & & \end{array}$$

where each $b_i(G_j) = 0$ except the values listed above.

Proof of (i) .

(**A**). Claim that $E(G_n^0) < E(G_1)$.

Note that $b_3(G_n^0) = (-1)a_3 = -((-1)2^1 \times 4) = 8$, $b_4(G_n^0) = 4(n-6) + 12 - 6 = 4n - 18$, $b_l(G_n^0) = 0 (l \geq 5)$. By (1.1),

$$E(G_1) - E(G_n^0) = \frac{1}{\pi}\int_0^{\infty} \frac{dx}{x^2} \ln \frac{f(x)}{\left[1 + (n+3)x^2 + (4n-18)x^4\right]^2 + \left[8x^3\right]^2},$$

where $f(x) = \big[1+(n+3)x^2+(4n-6)x^4+(6n-26)x^6+(4n-27)x^8\big]^2$ $+\big[8x^3+24x^5+24x^7+8x^9\big]^2$.

Let

$$\begin{aligned} g(x) &= \big[1+(n+3)x^2+(4n-6)x^4+(6n-26)x^6+(4n-27)x^8\big]^2+\big[8x^3 \\ &\quad +24x^5+24x^7+8x^9\big]^2-\big[1+(n+3)x^2+(4n-18)x^4\big]^2-64x^6 \\ &= \big[2+2(n+3)x^2+(8n-24)x^4+(6n-26)x^6+(4n-27)x^8\big] \\ &\quad \times\big[12x^4+(6n-26)x^6+(4n-27)x^8\big] \\ &\quad +\big(8x^3+24x^5+24x^7+8x^9\big)^2-64x^6. \end{aligned}$$

Note that $(8n-24),(6n-26)$ and $(4n-27)$ are positive if $n\geq 9$. So $g(x)>0$ when $n\geqslant 9$ and $x>0$. Hence $E(G_n^0)<E(G_1)$ for $n\geqslant 8$.

(**B**). Note that G_j contains at least 9 vertices and since $b_i(G_j)\geq b_i(G_n^0)\geq 0$ $(j=1,\cdots,8)$ for $n\geq 9$, by using mimic proof of $E(G_n^0)<E(G_1)$, we could show $E(G_n^0)<E(G_j)(j=2,\cdots,8)$ for $n\geq 9$. So we omit the proof here. Hence $E(G_n^0)<E(G_j)$ $(j=1,\cdots,8)$ for $n\geqslant 9$.

Proof of (ii) . Let

$$E(G_j)-E(G_n^1)=\frac{1}{\pi}\int_0^\infty \frac{dx}{x^2}\ln\frac{f_j(x)}{f_g(x)},$$

where

$$\begin{aligned} f_1(x) &= \big[1+(n+3)x^2+(4n-6)x^4+(6n-26)x^6+(4n-27)x^8\big]^2 \\ &\quad +\big[8x^3+24x^5+24x^7+8x^9\big]^2, \\ f_2(x) &= \big[1+(n+3)x^2+(4n-7)x^4+(5n-23)x^6+(2n-16)x^8\big]^2 \\ &\quad +\big[8x^3+20x^5+12x^7\big]^2, \\ f_3(x) &= \big[1+(n+3)x^2+(4n-8)x^4+(4n-20)x^6\big]^2+\big[8x^3+16x^5\big]^2, \\ f_4(x) &= \big[1+(n+3)x^2+(4n-8)x^4+(3n-12)x^6\big]^2+\big[8x^3+14x^5+6x^7\big]^2, \\ f_5(x) &= \big[1+(n+3)x^2+(4n-9)x^4+(3n-15)x^6\big]^2+\big[8x^3+12x^5\big]^2, \\ f_6(x) &= \big[1+(n+3)x^2+(4n-9)x^4+(3n-15)x^6\big]^2 \\ &\quad +\big[8x^3+(2n-2)x^5+(2n-12)x^7\big]^2, \\ f_7(x) &= \big[1+(n+3)x^2+(4n-15)x^4+(n-5)x^6\big]^2+\big[8x^3+(2n-6)x^5\big]^2, \\ f_8(x) &= \big[1+(n+3)x^2+(4n-16)x^4+(2n-10)x^6\big]^2+\big[8x^3+8x^5\big]^2, \\ f_g(x) &= \big[1+(n+3)x^2+(5n-35)x^4\big]^2. \end{aligned}$$

Using case by case checking, it is easy to see that $f_j(x)-f_g(x)\geq 0$ $(j=1,\cdots,8)$, where $9\leq n\leq 18$ and $x>0$. Hence $E(G_n^1)<E(G_j)$ for $9\leq n\leq 18$. □

Proposition 2.5. (i) $E(G_n^0)<E(G_n^1)$ *for* $n\geqslant 18$.

(ii) $E(G_n^1) < E(G_n^0)$ *for* $9 \leqslant n \leqslant 17$.

Proof. By Sachs theorem we can obtain $b_3(G_n^0) = 8, b_4(G_n^0) = 4n - 18$ and $b_i = 0$ for $i \geqslant 5$. Similarly, for G_n^1, we obtain $b_3(G_n^1) = 0, b_4(G_n^1) = 5n - 35$ and $b_i(G_n^1) = 0$ for $i \geqslant 5$, and so by (1.1),

$$E(G_n^1) - E(G_n^0) = \frac{1}{\pi}\int_0^\infty \frac{dx}{x^2}\ln\frac{\left[1+(n+3)x^2+(5n-35)x^4\right]^2}{\left[1+(n+3)x^2+(4n-18)x^4\right]^2+64x^6}.$$

To prove (i), let

$$\begin{aligned} f(x) &= \left[1+(n+3)x^2+(5n-35)x^4\right]^2 - \left[1+(n+3)x^2+(4n-18)x^4\right]^2 \\ &\quad -64x^6 = \left[(2+2(n+3)x^2+(9n-53)x^4)\right]\left[(n-17)x^4\right] - 64x^6. \end{aligned}$$

It follows that $f(x) > 0$ for $n \geqslant 19$. Hence $E(G_n^0) < E(G_n^1)$ for $n \geqslant 19$.

By direct calculation (rounded to four decimal places), we have $E(G_{18}^1) = 11.9720, E(G_{18}^0) = 11.9595$. Thus $E(G_n^0) < E(G_n^1)$ for $n \geq 18$.

To prove (ii), let

$$\begin{aligned} f^*(x) &= \left[1+(n+3)x^2+(4n-18)x^4\right]^2 + 64x^6 \\ &\quad -\left[1+(n+3)x^2+(5n-35)x^4\right]^2 \\ &= \left[(2+2(n+3)x^2+(9n-53)x^4)\right]\left[(17-n)x^4\right] + 64x^6. \end{aligned}$$

It follows that $f^*(x) \geq 0$ for $9 \leq n \leq 17$. Hence $E(G_n^1) < E(G_n^0)$ for $9 \leq n \leq 17$.

$\square$

By combining Propositions 2.3 and 2.5 and Lemma 2.4, we obtain the following main results of this paper.

Theorem 2.6. (i) G_n^1 *has minimal energy in* $\mathscr{G}_n$ *for* $9 \leqslant n \leqslant 17$.
(ii) G_n^0 *has minimal energy in* $\mathscr{G}_n$ *for* $n \geqslant 18$.

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