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On bicyclic graphs with minimal energies

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The energy of a graph is defined as the sum of the absolute values of all the eigenvalues of the graph. Let $G(n)$ be the class of bicyclic graphs G on n vertices and containing no disjoint odd cycles of lengths k and l with $k + l \equiv 2 \pmod 4$. In this paper, the graphs in $G(n)$ with minimal, second-minimal and third-minimal energies are determined.

KEY WORDS: energy, bicyclic graph, characteristic polynomial, eigenvalue

AMS subject classification: 05C50, 05C35

1. Introduction

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

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

The roots $\lambda_1, \lambda_2, \ldots, \lambda_n$ of $\phi(G, \lambda) = 0$ are called the eigenvalues of G. Since $A(G)$ is symmetric, all the eigenvalues of G are real.

The energy of G, denoted $E(G)$, is then defined as $E(G) = \sum_{i=0}^{n} |\lambda_i|$. It is known that [1] $E(G)$ can be expressed as the Coulson integral formula

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

Since the energy of a graph can be used to approximate the total π-electron energy of the molecule, it has been intensively studied. For a survey of the mathematical properties and results on $E(G)$, see the recent review [2].

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Many results on the minimal energy have been obtained for various classes of graphs, (see, for example, [3–5]). In [6], Caporossi et al. gave the following conjecture.

Conjecture 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 vertices for $e \leqslant n + \lfloor (n-7)/2 \rfloor$, 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 $e = n-1, 2(n-1)$ [6, Theorem 1], and when $e = n$ [7]. In this paper, we consider the above conjecture for the case $e = n+1$.

A connected graph with n vertices and $e = n+1$ edges is called a bicyclic graph. Let $G(n)$ be the class of bicyclic graphs G with n vertices and containing no disjoint odd cycles of lengths k and l with $k + l \equiv 2 \pmod 4$. Let $S_n^{3,3}$ be the graph formed by joining $n-4$ pendant vertices to a vertex of degree three of the $K_4 - e$, and $S_n^{4,4}$ be the graph formed by joining $n-5$ pendant vertices to a vertex of degree three of the complete bipartite graph $K_{2,3}$. Let $S_n'^{3,3}$, $S_n'^{4,4}$ be, respectively, the graph formed from $S_n^{3,3}$, $S_n^{4,4}$ by moving a pendant edge to the vertex of degree three. See figure 1 for these graphs. Hou [8] has reported that $S_n^{4,4}$ has the minimal energy among all n-vertex connected bicyclic graphs with at most one odd cycle. Note that the class of bicyclic graph with n vertices and at most one odd cycle is a proper subset of $G(n)$. In this paper, we show that $S_n^{3,3}$, $S_n^{4,4}$, $S_n'^{3,3}$ have, respectively, minimal, second-minimal and third-minimal energies in $G(n)$.

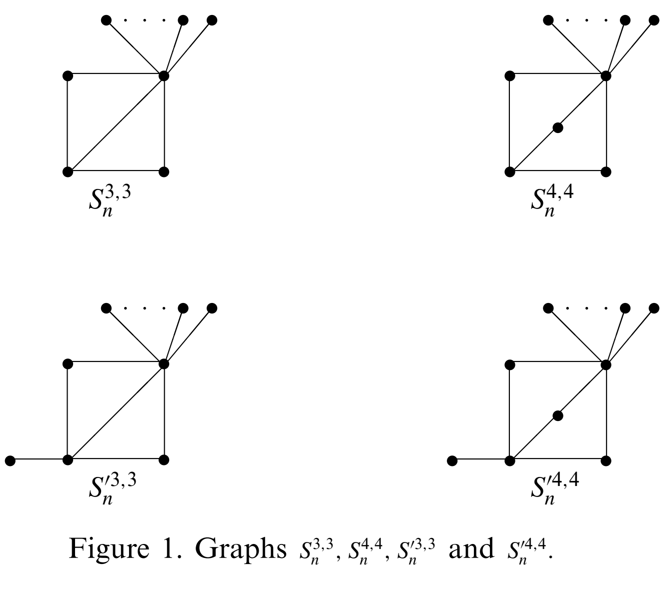

Figure 1. Graphs $S_n^{3,3}$, $S_n^{4,4}$, $S_n'^{3,3}$ and $S_n'^{4,4}$.

2. Main result

Let G be a graph with characteristic polynomial $\phi(G,\lambda) = \sum_{i=0}^{n} a_i \lambda^{n-i}$. Sachs theorem states that [1,9] 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 $a_0 = 1$. Let $b_{2i}(G) = (-1)^i a_{2i}$ and $b_{2i+1}(G) = (-1)^i a_{2i+1}$ for $0 \leqslant i \leqslant \lfloor n/2 \rfloor$. Clearly, $b_0(G) = 1$ and $b_2(G)$ equals the number of edges of G.

A graph G contains H means that G contains a subgraph that is isomorphic to H.

Lemma 1. (i) If $G \in G(n)$, then $b_{2i}(G) \geqslant 0$ for $1 \leqslant i \leqslant \lfloor n/2 \rfloor$.

(ii) If $G \in G(n)$ contains $K_4 - e$, then $b_{2i+1}(G) \geqslant 0$ for $1 \leqslant i \leqslant \lfloor n/2 \rfloor$.

Proof. Let L_i be the set of Sachs graphs of G with i vertices. Let $L_i^{(1)}$ be the set of graphs with no cycles in L_i, and $L_i^{(2)} = L_i \setminus L_i^{(1)}$. Note that $G \in G(n)$ has exactly two or three distinct cycles, and at most two odd cycles.

(i) By Sachs theorem,

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

If G has at most one odd cycle, then [10] $b_{2i}(G) \geqslant 0$. So we need only to consider the case when $G \in G(n)$ has exactly two odd cycles. If every S in L_{2i} has no cycles, then $p(S) = i$, $b_{2k}(G) = \sum_{S \in L_{2i}^{(1)}} 1 \geqslant 0$. Suppose some S_0 in L_{2i} contains at least one cycle C_s with length s. If s is odd, then S_0 contains exactly two disjoint odd cycles with lengths, say, s and t. Since $G \in G(n)$, we have $s + t \equiv 0 \pmod 4$, $p(S) + i = 2 + [2i - (s+t)]/2 + i \equiv 0 \pmod 2$, and then

$$b_{2i}(G) = \sum_{S \in L_{2i}^{(1)}} 1 + 4 \sum_{S \in L_{2i}^{(2)}} 1 \geqslant 0.$$

If s is even, then it is easy to see that $|L_{2i}^{(1)}| \geqslant 2|L_{2i}^{(2)}|$ and so

$$b_{2i}(G) = \sum_{S \in L_{2i}^{(1)}} 1 + \sum_{S \in L_{2i}^{(2)}} 2(-1)^{s-1} \geqslant 0.$$

(ii) If $G \in G(n)$ contains $K_4 - e$, then $L^{(1)}_{2i+1} = \emptyset$, any $S \in L^{(2)}_{2i+1}$ must contain a unique triangle, $p(S) = 1 + (2i + 1 - 3)/2 = i, c(S) = 1$, and so

$$b_{2i+1}(G) = 2 \sum_{S \in L^{(2)}_{2i+1}} 1 \geqslant 0. \qquad \square$$

In view of lemma 1, a quasi-order relation is introduced (see [3]).

(i) Let G_1, G_2 be the graphs of $G(n)$ containing $K_4 - e$. If $b_i(G_1) \geqslant b_i(G_2)$ holds for all $i \geqslant 0$, we say that G_1 is not less than G_2, written as $G_1 \succeq G_2$.

(ii) Let G_1 be any graph in $G(n)$, and $G_2 = S^{4,4}_n$. Similarly, we also write $G_1 \succeq G_2 = S^{4,4}_n$, if $b_{2i}(G_1) \geqslant b_{2i}(G_2)$ holds for all $i \geqslant 0$.

In either case, if $G_1 \succeq G_2$ and there exists on i such that $b_i(G_1) > b_i(G_2)$, then we write $G_1 \succ G_2$. Obvious, from (1) and lemma 1, we have the following increasing property on E:

$$G_1 \succ G_2 \Rightarrow E(G_1) > E(G_2). \tag{2}$$

Lemma 2. Let G be a graph with n vertices and let uv be a pendant edge of G with pendant vertex v. Then for $2 \leqslant i \leqslant n$,

$$b_i(G) = b_i(G - v) + b_{i-2}(G - u - v).$$

Proof. Since uv is a pendant edge of G with pendant vertex v, we have [9]

$$\phi(G, \lambda) = \lambda\phi(G - v, \lambda) - \phi(G - u - v, \lambda),$$

from which the result follows easily. $\square$

Let $m(G, 2)$ be 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 3. Let G be any graph. Then $b_4(G) = m(G, 2) - 2l$, where l is the number of quadrangles in G.

Proof. By Sachs theorem,

$$b_4(G) = \left| \sum_{S \in L_4} (-1)^{p(S)} 2^{c(S)} \right| = m(G, 2) - 2l$$

since any $S \in L_4$ is either $2K_2$ or a quadrangle. $\square$

Lemma 4. Let $G \in G(n)$. If $b_4(G) > b_4(S_n^{4,4}) = 3n - 15$, then $G \succ S_n^{4,4}$.

Proof. It is easy to see that $b_0(G) = b_0(S_n^{4,4})$, $b_2(G) = b_2(S_n^{4,4}) = n+1$, $b_4(S_n^{4,4}) = 3n - 15$, and $b_i(S_n^{4,4}) = 0$ for $i = 1, 3$ or $i \geqslant 5$. Since $b_4(G) > 3n - 15$, we have $G \succ S_n^{4,4}$. □

Lemma 5. If $G \in G(n)$ does not contain $K_4 - e$ and $G \not\cong S_n^{4,4}$, then $G \succ S_n^{4,4}$.

Proof. Since $G \in G(n)$, G has either two or three distinct cycles. If G has three cycles, then any two must share common edges. We may choose two cycles of lengths of a and b with t common edges such that $a - t \geqslant t, b - t \geqslant t$. If G has exactly two cycles, suppose the lengths of the two cycles are a and b. Then in any case we choose two cycles C_a and C_b with lengths a and b, respectively. We will prove that $b_4(G) > b_4(S_n^{4,4})(= 3n - 15)$.

Case 1. C_a and C_b have no common vertices. Then $n - a - b \geqslant 0$. By induction on $n - a - b$. If $n - a - b = 0$, then by lemma 3,

$$\begin{aligned} b_4(G) &\geqslant m(G,2) - 4 \\ &= m(C_a, 2) + m(C_b, 2) + ab + (a + b - 4) - 4 \\ &= \tfrac{1}{2}[(a+b)^2 - (a+b) - 16] \end{aligned}$$

and so

$$b_4(G) - (3n - 15) \geqslant \frac{1}{2}(n^2 - 7n + 14) > 0.$$

It follows that $b_4(G) > 3n - 15$.

Suppose it is true for all graphs in this case with $n - a - b < p$ $(p \geqslant 1)$, and suppose $n - a - b = p$.

Subcase 1.1. There is no pendant edges in G. Then C_a connects C_b by a path with length $p + 1$. By lemma 3,

$$\begin{aligned} b_4(G) &\geqslant m(G,2) - 4 \\ &= m(C_a, 2) + m(C_b, 2) + m(P_{p+2}, 2) + (a-2)(n+1-a) + 2(n-a) \\ &\quad + (b-2)(n+1-a-b) + 2(n-a-b) - 4 \\ &= \tfrac{1}{2}[n^2 - n + 2(a+b)^2 - 16] + a - 4 \end{aligned}$$

and so

$$b_4(G) - (3n - 15) \geqslant \frac{1}{2}[n^2 - 7n + 2(a+b)^2 + 2a + 6] > 0$$

and hence $b_4(G) > 3n - 15$.

Subcase 1.2. uv is a pendant edge of G with pendant vertex v. By lemma 2,

$$\begin{aligned} b_4(G) &= b_4(G - v) + b_2(G - u - v), \\ b_4(S_n^{4,4}) &= b_4(S_{n-1}^{4,4}) + b_2(K_{1,3}). \end{aligned}$$

By induction hypothesis, $b_4(G-v) \geqslant b_4(S_{n-1}^{4,4})$. Since G contains no K_4-e, $b_2(G-u-v) > 3 = b_2(K_{1,3})$. We have $b_4(G) > b_4(S_n^{4,4}) = 3n-15$.

By combining subcases 1.1 and 1.2, we have prove that in case 1, $b_4(G) > b_4(S_n^{4,4}) = 3n-15$.

Case 2. C_a and C_b have at least one common vertex and t ($t \geqslant 0$) common edges. Then $n-a-b+t \geqslant -1$. We use induction on $n-a-b+t$.

If $n-a-b+t = -1$, then G contains no vertices except vertices in the two cycles. There are four subcases.

Subcase 2.1. $t=0$. Then $n = a+b-1$. By lemma 3

$$\begin{aligned} b_4(G) &\geqslant m(G,2) - 4 \\ &= m(C_a,2) + m(C_b,2) + a(b-2) + 2(a-2) - 4 \\ &= \tfrac{1}{2}[(a+b)^2 - 3(a+b) - 16] \end{aligned}$$

and since $a+b \geqslant 6$, we have

$$b_4(G) - (3n-15) \geqslant \frac{1}{2}[(a+b)^2 - 9(a+b) + 20] > 0.$$

Subcase 2.2. $t=1$. Then $n = a+b-2$. If G contains quadrangles, then either $n=6$,

$$b_4(G) = 7 > 3 = b_4(S_6^{4,4})$$

or $n = b+2$, $b \neq 4$,

$$\begin{aligned} b_4(G) &= b - 2 + \tfrac{1}{2}(b+2)(b-1) - 2 \\ &> 3(b+2) - 15 \\ &= b_4(S_{b+2}^{4,4}, 2). \end{aligned}$$

Suppose G does not contain quadrangles. By lemma 3,

$$\begin{aligned} b_4(G) &= m(G,2) \\ &= a+b-6+m(C_{a+b-2},2), \\ &= a+b-6+\tfrac{1}{2}[(a+b-2)(a+b-5)]. \end{aligned}$$

Note that G does not contain quadrangles or K_4-e. We have $a+b \geqslant 6$ and hence

$$b_4(G) - (3n-15) = \frac{1}{2}[(a+b)^2 - 11(a+b) + 40] > 0.$$

Subcase 2.3. $t=2$. Then $n = a+b-3$. If G contains a quadrangle, let $a=4$. Then $b \neq 4$ since $G \ncong S_n^{4,4}$. By lemma 3,

$$b_4(G) = 2(b-2) + b(b-3)/2 - 2$$

and so

$$b_4(G) - b_4(S_n^{4,4}) = \frac{1}{2}(b^2 - 5b + 12) > 0.$$

If G does not contain quadrangles, then by lemma 3

$$b_4(G) = m(G, 2) = 2(a + b - 6) + m(C_{a+b-4}, 2)$$

and so

$$b_4(G) - b_4(S_n^{4,4}) = \frac{1}{2}[(a + b)^2 - 13(a + b) + 52)] > 0.$$

Subcase 2.4. $t \geqslant 3$. Note that $a, b \geqslant 2t$. Then $n = a+b-t-1$, by lemma 3

$$\begin{aligned} b_4(G) &= m(G, 2) \\ &= m(P_{t+1}, 2) + 2(a + b - 2t - 2) \\ &\quad +(t - 2)(a + b - 2t) + m(C_{a+b-2t}, 2) \end{aligned}$$

and so

$$\begin{aligned} b_4(G) - b_4(S_n^{4,4}) &= \frac{1}{2}[(a + b)^2 - (2t + 9)(a + b) + t^2 + 9t + 30] \\ &= \frac{1}{2}[(a + b) - (t + 3)][(a + b) - (t + 6)] + 6 > 0. \end{aligned}$$

By combining subcases 2.1–2.4, we have shown that in case 2, $b_4(G) > b_4(S_n^{4,4})$ if $n - a - b + t = -1$. Suppose that it is true for $n - a - b + t < p$ ($p \geqslant 0$), and that $n - a - b + t = p$. Then G must contain a pendant edges uv with v a pendant vertex. By lemma 2,

$$b_4(G) = b_4(G - v) + b_2(G - u - v),$$

$$b_4(S_n^{4,4}) = b_4(S_{n-1}^{4,4}) + b_2(K_{1,3}).$$

By induction hypothesis, $b_4(G - v) \geqslant b_4(S_{n-1}^{4,4})$. Since G does not contain $K_4 - e$, $b_2(G - u - v) > 3 = b_2(K_{1,3})$. So $b_4(G) > b_4(S_{a+b-t-1}^{4,4})$. Now we have have shown that in case 2, $b_4(G) > b_4(S_n^{4,4}) + 3n - 15$.

By combining cases 1 and 2, and by lemma 4, this theorem follows. □

Similarly, we have

Lemma 6. If $G \in G(n)$ does not contain $K_4 - e$, and $G \ncong S_n^{4,4}, S_n'^{4,4}$, then $G \succ S_n'^{4,4}$.

Lemma 7. If G contains $K_4 - e$, and $G \ncong S_n^{3,3}$, then $G \succ S_n^{3,3}$.

Proof. We will show $b_i(G) \geqslant b_i(S_n^{3,3})$ using induction on n. If $n = 4$, the theorem holds. Suppose it is true for $n < p$ ($p \geqslant 5$), and let $n = p$. Then G contains a pendant edge uv with pendant vertex v. By lemma 2,

$$\begin{aligned} b_i(G) &= b_i(G - v) + b_{i-2}(G - u - v), \\ b_i(S_n^{3,3}) &= b_i(S_{n-1}^{3,3}) + b_{i-2}(P_3). \end{aligned}$$

By induction hypothesis, $b_i(G-v) \geqslant b_i(S_{n-1}^{3,3})$. On the other hand, $b_{i-2}(G-u-v) \geqslant b_{i-2}(P_3)$ since

$$b_{i-2}(G - u - v) = \begin{cases} 1, & i - 2 = 0, \\ > 2, & i - 2 = 2, \\ \geqslant 0, & \text{otherwise} \end{cases}$$

and

$$b_{i-2}(P_3) = \begin{cases} 1, & i - 2 = 0, \\ 2, & i - 2 = 2, \\ 0, & \text{otherwise.} \end{cases}$$

Thus $b_i(G) \geqslant b_i(S_n^{3,3})$ holds for all i. Since $G \ncong S_n^{3,3}$, from the above argument, we see that $b_{i_0}(G) > b_{i_0}(S_n^{3,3})$ for some i_0. Now the theorem follows. □

Similarly, we have

Lemma 8. If $G \in G(n)$ contains $K_4 - e$, and $G \ncong S_n^{3,3}, S_n'^{3,3}$, then $G \succ S_n'^{3,3}$.

Lemma 9. $E(S_n'^{4,4}) > E(S_n'^{3,3}) > E(S_n^{4,4} > E(S_n^{3,3})$ for $n \geqslant 9$.

Proof. Note that

$$\begin{aligned} \phi(S_n'^{3,3}, \lambda) &= \lambda^n - (n+1)\lambda^{n-2} - 4\lambda^{n-3} + (3n - 13)\lambda^{n-4}, \\ \phi(S_n'^{4,4}, \lambda) &= \lambda^n - (n+1)\lambda^{n-2} + (4n - 21)\lambda^{n-4}, \\ \phi(S_n^{3,3}, \lambda) &= \lambda^n - (n+1)\lambda^{n-2} - 4\lambda^{n-3} + (2n - 8)\lambda^{n-4}, \\ \phi(S_n^{4,4}, \lambda) &= \lambda^n - (n+1)\lambda^{n-2} + (3n - 15)\lambda^{n-4}. \end{aligned}$$

From equation (1), we have

$$E(S_n'^{4,4}) - E(S_n'^{3,3}) = \frac{1}{\pi}\int_0^{+\infty} \frac{1}{x^2} \ln \frac{[1 + (n+1)x^2 + (4n - 21)x^4]^2}{[1 + (n+1)x^{-2} + (3n - 13)x^4]^2 + 16x^6} \mathrm{d}x.$$

Let

$$\begin{aligned} f(x) &= [1 + (n+1)x^2 + (4n - 21)x^4]^2 \\ &\quad -[1 + (n+1)x^{-2} + (3n - 13)x^4]^2 - 16x^6 \\ &= (n - 8)(7n - 34)x^8 + 2(n^2 - 7n + 16)x^6 + 2(n - 8)x^4. \end{aligned}$$

Then $f(x) > 0$ for $n \geqslant 9$. So $E(S_n'^{4,4}) > E(S_n'^{3,3})$. Similarly, we may get $E(S_n'^{3,3}) > E(S_n^{4,4}) > E(S_n^{3,3})$. □

Combining lemmas 5–9, and using the increasing property (2) on the energy, we obtain the following main result of this paper.

Theorem 1. $S_n^{3,3}$, $S_n^{4,4}$, $S_n'^{3,3}$ have, respectively, minimal, second-minimal and third-minimal energies in $G(n)$.

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References

[1] I. Gutman and O.E. Polansky, *Mathematicl Concepts in Organic Chemistry* (Springer -Verlag, Berlin, 1986).
[2] I. Gutman, in: *Algebraic Combinatorics and Applications*, eds. A. Betten, A. Kohnert, R. Laue and A. Wassermann (Springer-Verlag, Berlin, 2001), pp. 196–211.
[3] I. Gutman, Theoret. Chim. Acta (Berlin) 45 (1977) 79–87.
[4] F.J. Zhang and H. Li, Discrete Appl. Math. 92 (1999) 71–84.
[5] J. Rada and A. Tineo, Linear Algebra Appl. 372 (2003) 333–344.
[6] G. Caporossi, D. Cvetković, I. Gutman and P. Hansen, J. Chem. Inf. Comput. Sci. 39 (1999) 984–996.
[7] Y. Hou, J. Math. Chem. 29 (2001) 163–168.
[8] Y. Hou, Linear Multilinear Algebra 49 (2001) 347–354.
[9] D. Cvetkoić, M. Doob and H. Sachs, *Spectra of Graphs–Theory and Applications* (Academic Press, New York, 1980).
[10] I. Gutman and N. Tronajstić, J. Chem. Phys. 64 (1976) 4921–4925.