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MINIMAL ENERGIES OF BIPARTITE BICYCLIC GRAPHS

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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 $B(n)$ be the class of bipartite bicyclic graphs on n vertices containing a cycle with length congruent to 2 modulo 4. We determine respectively the graphs with minimal energies in the class of graphs in $B(n)$ with exactly three cycles, in the class of graphs in $B(n)$ with exactly two cycles of a common vertex, and in the class of graphs in $B(n)$ with exactly two vertex-disjoint cycles.

INTRODUCTION

We consider simple graphs. Let G be a graph on n vertices. The characteristic polynomial of G is

$$\phi(G, x) = \det[xI - A(G)],$$

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where I is the identity matrix of order n and $A(G)$ is the adjacency matrix of G. The roots $\lambda_1, \lambda_2, \cdots, \lambda_n$ of $\phi(G, x) = 0$ are called the eigenvalues of G [1]. Since $A(G)$ is symmetric, all the eigenvalues of G are real. The energy [2] of G, denoted by $E(G)$, is then defined as

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

In chemistry, the energy of a molecular graph can be used to approximate the total π-electron energy of the molecule represented by that graph. For more details, see the book [3] and the recent reviews [4, 5].

Let G be a bipartite graph on n vertices. The characteristic polynomial of G can be written as

$$\phi(G, x) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k b_k(G) x^{n-2k},$$

where $b_k(G) \geq 0$ (see [1, 3]). The energy of G can be expressed as the Coulson integral formula [3]

$$E(G) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \log \left[\sum_{k=0}^{\lfloor n/2 \rfloor} b_k(G) x^{2k} \right] \mathrm{d}x. \tag{1}$$

Let $b_k(G) = 0$ if $k > \lfloor n/2 \rfloor$. In view of the expression for $\phi(G, x)$, a quasi–order relation can be introduced over the class of all bipartite graphs [6]: For bipartite graphs G_1 and G_2, if $b_k(G_1) \geq b_k(G_2)$ for all $k \geq 0$, then we write $G_1 \succeq G_2$. If $G_1 \succeq G_2$ and there is a k_0 such that $b_{k_0}(G_1) > b_{k_0}(G_2)$, then we write $G_1 \succ G_2$. From (1) we have the following increasing property of energy:

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

A connected graph with n vertices and n edges is called a unicyclic graph, and a connected graph with n vertices and $n + 1$ edges is called a bicyclic graph.

From a chemical point of view, it is of greatest interest to find the extremal values of the energy for significant classes of graphs. For instance, Gutman [6] determined the trees with minimal and maximal energies. Hou [7] determined the unicyclic graphs with minimal energy. Hou [8], Zhang and Zhou [9, 10] studied the minimal energies of bicyclic graphs. More results in this direction can be found in [11–27].

Let G be a bicyclic graph. The bicyclic subgraph of G with no pendent vertices (i.e., vertices of degree one) is called the base graph of G, denoted by $\widehat{G}$. If $\widehat{G}$ contains exactly three cycles, then we say that G is a θ-based graph. If $\widehat{G}$ consists of two cycles with exactly one common vertex, then we say that G is a ∞_1-based graph. If $\widehat{G}$ contains two vertex-disjoint cycles, then we say that G is a ∞_2-based graph.

If an edge is introduced between one end vertex of a path and a vertex v of a graph G, we say that the path is attached to vertex v of G. Let B be the graph with 6 vertices formed by identifying an edge of two quadrangles. Let B_n^1 be the graph formed by attaching $n-6$ pendent vertices to a vertex of degree two of B, B_n^2 be the graph formed by attaching $n-6$ pendent vertices to a vertex of degree three of B, B_n^3 be the graph formed by identifying a vertex of a hexagon and a vertex of a quadrangle, and attaching $n-9$ pendent vertices to this common vertex, B_n^4 be the graph formed by introducing an edge between a vertex of a hexagon and a vertex of a quadrangle, and attaching $n-10$ pendent vertices to the vertex of degree three in the hexagon. See Fig. 1 for the graphs B_n^i, $i = 1, 2, 3, 4$.

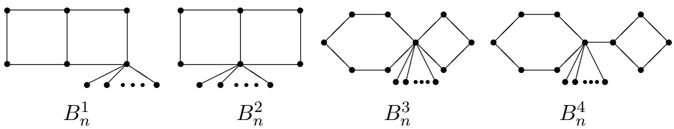


Fig. 1. Graphs B_n^i, $i = 1, 2, 3, 4$.

By a result in [9], the graph formed by attaching $n-5$ pendent vertices to a vertex of degree three of the complete bipartite graph $K_{2,3}$ is the unique graph with minimal energy in the class of n-vertex bipartite bicyclic graphs. In [10], it is shown that the graph formed by attaching $n-7$ pendent vertices to the vertex of degree four of the graph consisting of two quadrangles with exactly one common vertex is the unique graph with minimal energy in the class of n-vertex bipartite bicyclic graphs of exactly two cycles. Note that in both extremal graphs all cycle lengths are $\equiv 0 \pmod 4$. Let $B(n)$ be the class of n-vertex bipartite bicyclic graphs containing a cycle of length $\equiv 2 \pmod 4$. Let $B_\theta(n)$, $B_{\infty_1}(n)$ and $B_{\infty_2}(n)$ be respectively the class of θ-, ∞_1-, and ∞_2-based graphs in $B(n)$. It is a natural question to ask which graphs achieve the minimal energy in $B_\theta(n)$, $B_{\infty_1}(n)$ and $B_{\infty_2}(n)$, respectively. The main result of this work is that in the three classes $B_\theta(n)$, $B_{\infty_1}(n)$ and $B_{\infty_2}(n)$, the graphs B_n^1 or B_n^2, B_n^3, and B_n^4 have minimal energy, respectively. A more precise statement of our results is given in Theorem 4.

PRELIMINARIES

Let G be a bipartite graph on n vertices. Sachs theorem states that [1, 3] for $k \geq 1$,

$$(-1)^k b_k(G) = \sum_{S \in L_{2k}} (-1)^{p(S)} 2^{c(S)},$$

where L_{2k} denotes the set of Sachs graph of G with $2k$ vertices, in which every component is either a complete graph with two vertices or a cycle, $p(S)$ is the number of components and $c(S)$ is the number of cycles in S. Clearly, $b_0(G) = 1$, $b_1(G)$ equals the number of edges of G. For convenience, let $b_k(G) = 0$ if $k < 0$.

Let $m(G,k)$ be number of k-matchings of G. If G is acyclic, then $b_k(G) = m(G,k)$ for all k (see [1, 3]). Let P_n and C_n be respectively the path and cycle on n vertices. Note that $m(P_n, 2) = \frac{(n-2)(n-3)}{2}$ and $m(C_n, 2) = \frac{n(n-3)}{2}$.

If G is a bipartite graph containing exactly one quadrangle, then by Sachs theorem, we have $b_2(G) = m(G,2) - 2$, and $b_3(G) \geq m(G,3) - 2m(G - C_4, 1)$.

Let G be a bipartite graph. Let $C(uv)$ denote the set of cycles containing the edge uv in G. By [1], we have $\phi(G,x) = \phi(G-uv,x) - \phi(G-u-v,x) - 2\sum_{C \in C(uv)} \phi(G-C,x)$, from which the following result follows easily.

Lemma 1. *Let G be a bipartite graph.*

(i) If uv is a bridge in G, then

$$b_k(G) = b_k(G - uv) + b_{k-1}(G - u - v),$$

in particular, if u is a pendent vertex, being adjacent to v, then

$$b_k(G) = b_k(G - u) + b_{k-1}(G - u - v).$$

(ii) If uv is an edge on some cycle, then

$$b_k(G) = b_k(G - uv) + b_{k-1}(G - u - v) - 2 \sum_{C_r \in C(uv)} (-1)^{\frac{r}{2}} b_{k-\frac{r}{2}}(G - C_r).$$

From Lemma 1 (i), we have

Lemma 2. *Let G be a bipartite graph. If H is obtained from G by deleting some bridges and/or pendent vertices, then $b_k(G) \geq b_k(H)$ for all $k \geq 0$.*

Lemma 3. [3] *For $1 \leq i < \lfloor \frac{n}{2} \rfloor$, $P_n \succeq P_{2i} \cup P_{n-2i} \succeq P_1 \cup P_{n-1}$.*

Let U_n^r be the unicyclic graph formed by attaching the path P_{n-r} to a vertex of the cycle C_r. Let $U_{n,i}$ be the graph obtained from B_n^i by deleting an edge incident with the vertex of maximal degree and a vertex of degree 2 in the hexagon, where $i = 2, 3, 4$.

Lemma 4. *Let b be an even integer with $4 \leq b \leq n-1$ and $i = 2, 3, 4$, where $n \geq 7$ if $i = 2$, $n \geq 9$ if $i = 3$ and $n \geq 10$ if $i = 4$. Then $b_k(U_n^b) \geq b_k(U_{n,i})$ for $k = 2, 3, 4$.*

Proof. By Lemma 1,

$$\begin{aligned} b_k(U_n^4) &= b_k(P_n) + b_{k-1}(P_{n-4} \cup P_2) - 2b_{k-2}(P_{n-4}) \\ &= b_k(P_{n-1}) + b_{k-1}(P_{n-3}) + b_{k-2}(P_{n-4}) + b_{k-1}(P_{n-4}) \\ &\quad + b_{k-2}(P_{n-4}) - 2b_{k-2}(P_{n-4}) \\ &= b_k(P_{n-1}) + b_{k-1}(P_{n-3}) + b_{k-1}(P_{n-4}). \end{aligned}$$

Let $P_{n,i,s}$ be the tree obtained by attaching s pendent vertices to the i-th vertex of the path P_n labelled consecutively by $1, 2, \ldots, n$. Obviously, $P_{n,i,0} = P_n$. Similarly,

$$\begin{aligned} b_k(U_{n,2}) &= b_k(P_{6,1,n-7}) + b_{k-1}(P_4) + b_{k-1}(P_2) + b_{k-3}(P_1), \\ b_k(U_{n,3}) &= b_k(P_{8,3,n-9}) + b_{k-1}(P_{6,1,n-9}) + b_{k-1}(P_5), \\ b_k(U_{n,4}) &= b_k(P_{9,4,n-10}) + b_{k-1}(P_{7,2,n-10}) + b_{k-1}(P_{6,1,n-10}). \end{aligned}$$

Note that $b_k(P_n) \geq b_k(T)$ for any tree T with n vertices and all $k \geq 0$ (see [6]). By Lemma 2, we have $b_k(U_n^4) \geq b_k(U)$ for $k = 2, 3, 4$, where $U \in \{U_{n,2}, U_{n,3}, U_{n,4}\}$.

Suppose that $b \geq 6$. We need only to show that $b_k(U_n^b) \geq b_k(U_n^4)$ for $k = 2, 3, 4$.

First suppose that $(k, b) \neq (4, 8)$. Then for $k = 2, 3, 4$, by Lemma 1,

$$\begin{aligned} b_k(U_n^b) &= b_k(P_n) + b_{k-1}(P_{n-b} \cup P_{b-2}) - (-1)^{\frac{b}{2}} 2b_{k-\frac{b}{2}}(P_{n-b}) \\ &\geq b_k(P_n) + b_{k-1}(P_{n-b} \cup P_{b-2}) \\ &= b_k(P_{n-1}) + b_{k-1}(P_{n-2}) + b_{k-1}(P_{n-b} \cup P_{b-2}). \end{aligned}$$

By Lemma 3, we have $b_{k-1}(P_{n-2}) \geq b_{k-1}(P_{n-3})$, $b_{k-1}(P_{n-b} \cup P_{b-2}) \geq b_{k-1}(P_{n-3}) \geq b_{k-1}(P_{n-4})$. Then we have $b_k(U_n^b) \geq b_k(U_n^4)$.

Now suppose that $(k, b) = (4, 8)$. By Lemma 1, we have

$$\begin{aligned} b_4(U_n^8) &= b_4(P_n) + b_3(P_{n-8} \cup P_6) - 2 \\ &= b_4(P_{n-1}) + b_3(P_{n-2}) + b_3(P_{n-8} \cup P_6) - 2 \\ &= b_4(P_{n-1}) + b_3(P_{n-3}) + b_2(P_{n-4}) + b_3(P_{n-8} \cup P_6) - 2. \end{aligned}$$

By Lemma 3, $b_3(P_{n-8} \cup P_6) \geq b_3(P_{n-3}) \geq b_3(P_{n-4})$. Note that $b_2(P_{n-4}) \geq 2$. Thus $b_4(U_n^8) \geq b_4(U_n^4)$. $\square$

Lemma 5. *Let G_1, G_2 be two vertex-disjoint bipartite graphs with $|V(G_1)|+|V(G_2)| = n$. Then $b_k(G_1 \cup G_2) = \sum_{i=0}^{k} b_i(G_1) b_{k-i}(G_2)$ for $0 \leq k \leq \lfloor \frac{n}{2} \rfloor$.*

Proof. Let $|V(G_i)| = n_i$ for $i = 1, 2$. It is easy to see that

$$\begin{aligned}\phi(G_1 \cup G_2, x) &= \phi(G_1, x)\phi(G_2, x) \\ &= \left[\sum_{i=0}^{\lfloor n_1/2 \rfloor} (-1)^i b_i(G_1) x^{n_1-2i}\right]\left[\sum_{j=0}^{\lfloor n_2/2 \rfloor} (-1)^j b_j(G_2) x^{n_2-2j}\right] \\ &= \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k \left[\sum_{i=0}^{k} b_i(G_1) b_{k-i}(G_2)\right] x^{n-2k}.\end{aligned}$$

Now the result follows easily. □

Lemma 6. *Let a, b and n be integers, where $a \equiv 2 \pmod 4$, $a \geq 6$, b is even, $4 \leq b \leq n-1$. Let H be the graph formed by identifying the pendent vertex of U_n^b and a vertex of C_a. Then $b_k(U_n^b \cup C_a) \geq b_k(H)$ for all $k \geq 0$.*

Proof. Let u be the pendent vertex, being adjacent to v, in U_n^b. Let $U = U_n^b - u - v$. By Lemma 1,

$$\begin{aligned}b_k(C_a \cup U_n^b) &= b_k(C_a \cup U_{n-1}^b) + b_{k-1}(C_a \cup U), \\ b_k(H) &= b_k(C_a \cup U_{n-1}^b) + b_{k-1}(P_{a-1} \cup U).\end{aligned}$$

By Lemma 5, we have

$$\begin{aligned}b_{k-1}(C_a \cup U) &= \sum_{i=0}^{k-1} b_i(C_a) b_{k-i-1}(U), \\ b_{k-1}(P_{a-1} \cup U) &= \sum_{i=0}^{k-1} b_i(P_{a-1}) b_{k-i-1}(U).\end{aligned}$$

Note that $a \equiv 2 \pmod 4$. By Lemma 1 (ii), we have $b_i(C_a) \geq b_i(P_a) + b_{i-1}(P_{a-2}) \geq b_i(P_{a-1})$. It follows that $b_{k-1}(C_a \cup U) \geq b_{k-1}(P_{a-1} \cup U)$ for all $k \geq 0$. Thus the result follows. □

RESULTS

Now we consider minimal energies of the graphs in the class of $B_\theta(n)$, $B_{\infty_1}(n)$ and $B_{\infty_2}(n)$, respectively.

Theorem 1. *If $G \in B_\theta(n)$ and $G \neq B_n^1, B_n^2$, where $n \geq 8$, then $G \succ B_n^2$.*

Proof. Note that $b_k(B_n^2) = 0$ for $k \geq 4$. We will show that $b_k(G) \geq b_k(B_n^2)$ for $k = 2, 3$ and it is strict for $k = 2$. We use induction on n.

The graphs in $B_\theta(8)$ (except B_8^1, B_8^2) are shown in Fig. 2, and the b_2, b_3-values are listed below the corresponding graphs. Note that $b_2(B_8^2) = 15$ and $b_3(B_8^2) = 7$. It can be checked that the result is true for $n = 8$.

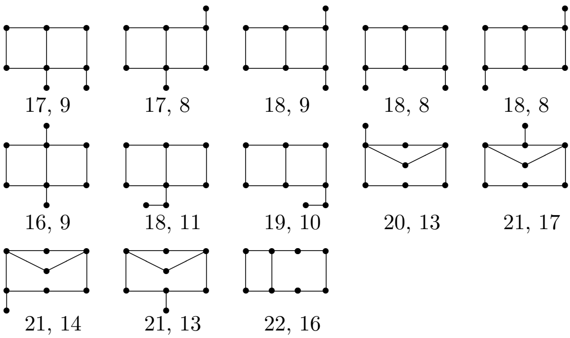


Fig. 2. Graphs in $B_\theta(8)$ (except B_8^1, B_8^2) and their b_2, b_3-values.

Suppose that $n \geq 9$ and the result is true for graphs with $n-1$ vertices. Let $G \in B_\theta(n)$. Then G contains three cycles, say C_a, C_b and C_c, where $a \equiv 2 \pmod 4$ and $b \leq c$.

Case 1. $\widehat{G} = G$. Let u be a vertex of degree three of G and v be its neighbor outside C_b. Since $n \geq 9$, we have $c \geq 6$. By Lemma 1 (ii),

$$\begin{aligned} b_k(G) &= b_k(U_n^b) + b_{k-1}(G-u-v) + 2b_{k-\frac{a}{2}}(G-C_a) - (-1)^{\frac{c}{2}} 2b_{k-\frac{c}{2}}(G-C_c) \\ &\geq b_k(U_n^b) + b_{k-1}(G-u-v), \\ b_k(B_n^2) &= b_k(U_{n,2}) + b_{k-1}(P_4) + 2b_{k-3}((n-6)P_1) - 2b_{k-2}(P_2) = b_k(U_{n,2}) + 1 \end{aligned}$$

for $k = 2, 3$. By Lemma 4, we have $b_k(U_n^b) \geq b_k(U_{n,2})$ for $k = 2, 3$. Note that $G-u-v$ is a tree. By Sachs theorem,

$$\begin{aligned} b_1(G-u-v) &= n-3 > 1, \\ b_2(G-u-v) &= m(G-u-v, 2) \geq m(P_{a-2}, 2) = \frac{(a-4)(a-5)}{2} \geq 1. \end{aligned}$$

Hence we have $b_k(G) \geq b_k(B_n^2)$ for $k = 2, 3$ and it is strict for $k = 2$.

Case 2. $\widehat{G} \neq G$. Since $G \neq B_n^1$, B_n^2, and $n \geq 9$, we can choose a pendent vertex u, being adjacent to v, in G such that $G - u \neq B_{n-1}^1$, B_{n-1}^2. By Lemma 1 (i),

$$\begin{aligned} b_k(G) &= b_k(G-u) + b_{k-1}(G-u-v), \\ b_k(B_n^2) &= b_k(B_{n-1}^2) + b_{k-1}(P_5) \end{aligned}$$

for $k = 2, 3$, where

$$b_{k-1}(P_5) = \begin{cases} 4, & \text{if } k = 2, \\ 3, & \text{if } k = 3. \end{cases}$$

By the induction hypothesis, $b_k(G - u) \geq b_k(B^2_{n-1})$ for $k = 2, 3$, and it is strict for $k = 2$. We need only to show that $b_{k-1}(G - u - v) \geq b_{k-1}(P_5)$ for $k = 2, 3$.

Subcase 2.1. $G-u-v$ contains $\widehat{G}$. By Lemma 2, we have $b_{k-1}(G-u-v) \geq b_{k-1}(\widehat{G})$. So by Sachs theorem,

$$\begin{aligned} b_1(G - u - v) &\geq b_1(C_a) = a > 4, \\ b_2(G - u - v) &\geq m(\widehat{G}, 2) - 4 \geq m(C_a, 2) - 4 = \frac{a(a-3)}{2} - 4 \geq 5 > 3. \end{aligned}$$

Subcase 2.2. $G - u - v$ contains exactly one cycle C. If C is a quadrangle, then $G-u-v$ contains a subgraph H which is a unicyclic graph with 6 vertices or $P_2 \cup U^4_5$, and so by Lemma 2,

$$\begin{aligned} b_1(G - u - v) &\geq b_1(H) = 6 > 4, \\ b_2(G - u - v) &\geq b_2(H) = m(H, 2) - 2 \geq 3. \end{aligned}$$

Otherwise, we have $C = C_r$ with $r \geq 6$, and by Sachs theorem,

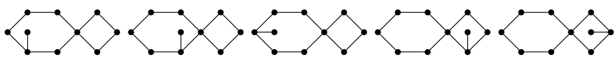
$$\begin{aligned} b_1(G - u - v) &= m(G - u - v, 1) \geq m(C_r, 1) \geq 6 > 4, \\ b_2(G - u - v) &= m(G - u - v, 2) \geq m(C_r, 2) = \frac{r(r-3)}{2} > 3. \end{aligned}$$

Subcase 2.3. $G - u - v$ is acyclic. Then P_5 is a subgraph of $G - u - v$. By Lemma 2, we have $b_{k-1}(G - u - v) \geq b_{k-1}(P_5)$ for $k = 2, 3$.

Combining Subcases 2.1–2.3, we have $b_{k-1}(G - u - v) \geq b_{k-1}(P_5)$ for $k = 2, 3$. Therefore $b_k(G) \geq b_k(B^2_n)$ for $k = 2, 3$ and it is strict for $k = 2$. Now the result follows. $\square$

Theorem 2. *If $G \in B_{\infty_1}(n)$ and $G \neq B^3_n$, where $n \geq 10$, then $G \succ B^3_n$.*

Proof. Note that $\phi(B^3_n, x) = x^n - (n+1)x^{n-2} + (6n - 25)x^{n-4} - (11n - 71)x^{n-6} + (6n - 46)x^{n-8}$. So $b_k(B^3_n) = 0$ for $k \geq 5$. We will show that $b_k(G) \geq b_k(B^3_n)$ for $k = 2, 3, 4$ and it is strict for $k = 2$. We use induction on n.



37, 43, 14   37, 45, 16   37, 43, 16   37, 47, 24   37, 45, 18

Fig. 3. Graphs in $B_{\infty_1}(10)$ (except B^3_{10}) and their b_2, b_3, b_4-values.

The graphs in $B_{\infty_1}(10)$ (except B_{10}^3) are shown in Fig. 3, and the b_2, b_3, b_4-values are listed below the corresponding graphs. Since the b_2, b_3, b_4-values of B_{10}^3 are respectively $35, 39, 14$, it can be checked that the result is true for $n = 10$.

Suppose that $n \geq 11$, and the result is true for all graphs with $n-1$ vertices. Let $G \in B_{\infty_1}(n)$ and $G \neq B_n^3$. Then G contains two cycles, say C_a and C_b, where $a \equiv 2 \pmod 4$.

Case 1. $\widehat{G} = G$. Then $n = a+b-1$, and either $a = 6$, $b \geq 6$ or $b = 4$, $a \geq 10$. By Lemma 1 (ii),

$$\begin{aligned} b_k(G) &= b_k(U_n^b) + b_{k-1}(P_{a-2} \cup P_{b-1}) + 2b_{k-\frac{a}{2}}(P_{b-1}) \\ &\geq b_k(U_n^b) + b_{k-1}(P_{a-2} \cup P_{b-1}), \\ b_k(B_n^3) &= b_k(U_{n,3}) + b_{k-1}(P_4 \cup P_3) + 2b_{k-3}(P_3), \end{aligned}$$

where it is easy to see that

$$b_{k-1}(P_4 \cup P_3) + 2b_{k-3}(P_3) = \begin{cases} 5, & \text{if } k = 2, \\ 9, & \text{if } k = 3, \\ 6, & \text{if } k = 4. \end{cases}$$

By Lemma 4, $b_k(U_n^b) \geq b_k(U_{n,3})$ for $k = 2, 3, 4$. Moreover, $b_{k-1}(P_{a-2} \cup P_{b-1}) = m(P_{a-2} \cup P_{b-1}, k-1)$ and so

$$\begin{aligned} b_1(P_{a-2} \cup P_{b-1}) &= a+b-5 = n-4 > 5, \\ b_2(P_{a-2} \cup P_{b-1}) &\geq (a-3)(b-2) > 9, \\ b_3(P_{a-2} \cup P_{b-1}) &\geq (b-2)m(P_{a-2}, 2) + (a-3)m(P_{b-1}, 2) \\ &= \frac{(a-4)(a-5)(b-2)}{2} + \frac{(a-3)(b-3)(b-4)}{2} > 6. \end{aligned}$$

Therefore, $b_k(G) > b_k(B_n^3)$ for $k = 2, 3, 4$.

Case 2. $\widehat{G} \neq G$.

Let G_0 be the graph obtained by attaching a pendent vertex to the pendent vertex of B_{10}^3. Note that

$$\begin{aligned} b_2(G_0) = 45, \quad b_3(G_0) = 68, \quad b_4(G_0) = 42, \\ b_2(B_{11}^3) = 41, \quad b_3(B_{11}^3) = 50, \quad b_4(B_{11}^3) = 20. \end{aligned}$$

If $G = G_0$, then the result follows.

Suppose that $G \neq G_0$. Then we can choose a pendent vertex u, being adjacent to v, in G such that $G - u \neq B_{n-1}^3$. By Lemma 1 (i),

$$\begin{aligned} b_k(G) &= b_k(G-u) + b_{k-1}(G-u-v), \\ b_k(B_n^3) &= b_k(B_{n-1}^3) + b_{k-1}(P_5 \cup P_3) \end{aligned}$$

for $k = 2, 3, 4$, and

$$b_{k-1}(P_5 \cup P_3) = \begin{cases} 6, & \text{if } k = 2, \\ 11, & \text{if } k = 3, \\ 6, & \text{if } k = 4. \end{cases}$$

By the induction hypothesis, $b_k(G-u) \geq b_k(B^3_{n-1})$ for $k = 2, 3, 4$, and it is strict for $k = 2$. It suffices to show that $b_{k-1}(G-u-v) \geq b_{k-1}(P_5 \cup P_3)$ for $k = 2, 3, 4$.

Subcase 2.1. $G-u-v$ contains $\widehat{G}$. By Lemma 2, $b_{k-1}(G-u-v) \geq b_{k-1}(\widehat{G})$, and then by Sachs theorem,

$$\begin{aligned} b_1(G-u-v) &\geq m(\widehat{G}, 1) = a + b > 6, \\ b_2(G-u-v) &\geq m(\widehat{G}, 2) - 2 \\ &= m(C_a, 2) + m(C_b, 2) + a(b-2) + 2(a-2) - 2 \\ &\geq a(b-2) + 2(a-2) - 2 > 11, \\ b_3(G-u-v) &\geq m(\widehat{G}, 3) - 2(a-2) \\ &\geq (b-2)m(C_a, 2) + (a-2)m(C_b, 2) - 2(a-2) \\ &= \frac{a(a-3)(b-2)}{2} + \frac{b(a-2)(b-3)}{2} - 2(a-2) \\ &\geq \frac{a(a-3)(b-2)}{2} > 6. \end{aligned}$$

Subcase 2.2. $G-u-v$ contains exactly one cycle C_r, $r \in \{a, b\}$. By Sachs theorem, $b_{k-1}(G-u-v) = m(G-u-v, k-1) + 2(-1)^{\frac{r}{2}-1} m(G-u-v-C_r, k-1-\frac{r}{2})$. Then

$$b_1(G-u-v) \geq a + b - 2 > 6.$$

Suppose that $k = 3, 4$. If $r \geq 6$, then $b_{k-1}(G-u-v) \geq m(G-u-v, k-1)$; if $r = 4$, then $b_{k-1}(G-u-v) = m(G-u-v, k-1) - 2m(G-u-v-C_4, k-3)$. In either case, we have $b_{k-1}(G-u-v) \geq m(P_{a-1}, k-1) + 2m(P_{a-1}, k-2)$. Thus

$$\begin{aligned} b_2(G-u-v) &\geq \frac{(a-3)(a-4)}{2} + 2(a-2) \geq 11, \\ b_3(G-u-v) &\geq (a-3)(a-4) \geq 6. \end{aligned}$$

Subcase 2.3 $G-u-v$ is acyclic. Then $P_5 \cup P_3$ is a subgraph of $G-u-v$. By Lemma 2, $b_{k-1}(G-u-v) \geq b_{k-1}(P_5 \cup P_3)$ for $k = 2, 3, 4$.

Combining Subcases 2.1–2.3, we have $b_{k-1}(G-u-v) \geq b_{k-1}(P_5 \cup P_3)$ for $k = 2, 3, 4$. Therefore $b_k(G) \geq b_k(B^3_n)$ for $k = 2, 3, 4$ and it is strict for $k = 2$. Now the result follows. $\square$

Theorem 3. *If $G \in B_{\infty_2}(n)$ and $G \neq B^4_n$, where $n \geq 11$, then $G \succ B^4_n$.*

Proof. Note that $\phi(B_n^4, x) = x^n - (n+1)x^{n-2} + (8n-41)x^{n-4} - (19n-139)x^{n-6} + (12n-98)x^{n-8}$. So $b_k(B_n^4) = 0$ for $k \geq 5$. We will show that $b_k(G) \geq b_k(B_n^4)$ for $k = 2, 3, 4$, and it is strict for $k = 3$. We use induction on n.

The graphs in $B_{\infty_2}(11)$ (except B_{11}^4) are shown in Fig. 4, and the b_2, b_3, b_4-values are listed below the corresponding graphs. Since the b_2, b_3, b_4-values of B_{11}^4 are respectively $47, 70, 34$, it can be checked that the result is true for $n = 11$.

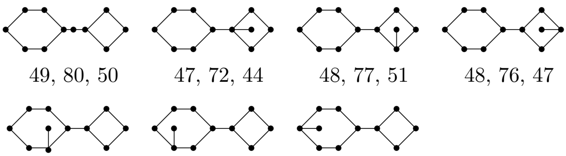


Fig. 4. Graphs in $B_{\infty_2}(11)$ (except B_{11}^4) and their b_2, b_3, b_4-values.

Suppose $n \geq 12$ and the result is true for all graph on $n-1$ vertices. Let $G \in B_{\infty_2}(n)$, and $G \neq B_n^4$. Then G contains two vertex-disjoint cycles, say C_a and C_b, where $a \equiv 2 \pmod 4$.

Suppose that $n = a + b$. Then G is formed by introducing an edge between a vertex in C_a and a vertex in C_b, where either $a = 6$, $b \geq 6$ or $b = 4$, $a \geq 10$. By Lemma 1 (ii),

$$\begin{aligned} b_k(G) &= b_k(U_n^b) + b_{k-1}(P_{a-2} \cup C_b) + 2b_{k-\frac{a}{2}}(C_b) \\ &\geq b_k(U_n^b) + b_{k-1}(P_{a-2} \cup C_b), \\ b_k(B_n^4) &= b_k(U_{n,4}) + b_{k-1}(P_4 \cup C_4) + 2b_{k-3}(C_4), \end{aligned}$$

where

$$b_{k-1}(P_4 \cup C_4) + 2b_{k-3}(C_4) = \begin{cases} 7, & \text{if } k = 2, \\ 15, & \text{if } k = 3, \\ 12, & \text{if } k = 4. \end{cases}$$

By Lemma 4, we know that $b_k(U_n^b) \geq b_k(U_{n,4})$ for $k = 2, 3, 4$. Moreover, by Sachs theorem,

$$\begin{aligned} b_1(P_{a-2} \cup C_b) &= n - 3 > 7, \\ b_2(P_{a-2} \cup C_b) &\geq m(P_{a-2} \cup C_b, 2) - 2 \\ &\geq m(P_{a-2}, 2) + m(C_b, 2) + (a-3)b - 2 \\ &\geq (a-3)b > 15, \end{aligned}$$

$$\begin{aligned}
b_3(P_{a-2}\cup C_b) &\geq m(P_{a-2}\cup C_b,3)-2(a-3)\\
&= bm(P_{a-2},2)+m(P_{a-2},3)+m(C_b,3)\\
&\quad +m(C_b,2)(a-3)-2(a-3)\\
&\geq bm(P_{a-2},2)+m(C_b,2)(a-3)-2(a-3)\\
&= \frac{(a-4)(a-5)b}{2}+(a-3)\left[\frac{b(b-3)}{2}-2\right]>12.
\end{aligned}$$

It follows that $b_{k-1}(P_{a-2}\cup C_b)>b_{k-1}(P_4\cup C_4)+2b_{k-3}(C_4)$ for $k=2,3,4$. Therefore $b_k(G)>b_k(B_n^4)$ for $k=2,3,4$.

Now suppose that $n>a+b$. By Lemma 1 (i),

$$b_k(B_n^4)=b_k(B_{n-1}^4)+b_{k-1}(P_5\cup C_4),$$

for $k=2,3,4$, and

$$b_{k-1}(P_5\cup C_4)=\begin{cases}8, & \text{if } k=2,\\ 19, & \text{if } k=3,\\ 12, & \text{if } k=4.\end{cases}$$

Case 1. $\widehat{G}=G$. By Lemma 1 (i),

$$b_k(G)=b_k(C_a\cup U_{n-a}^b)+b_{k-1}(P_{a-1}\cup U_{n-a-1}^b).$$

By Lemma 6 and the induction hypothesis, we have $b_k(C_a\cup U_{n-a}^b)\geq b_k(H)\geq b_k(B_{n-1}^4)$ for $k=2,3,4$, and $b_3(C_a\cup U_{n-a}^b)>b_3(B_{n-1}^4)$, where H is the graph obtained by identifying a vertex of C_a and the pendent vertex of U_{n-a}^b. Moreover, by Sachs theorem,

$$\begin{aligned}
b_1(P_{a-1}\cup U_{n-a-1}^b) &= n-3>8,\\
b_2(P_{a-1}\cup U_{n-a-1}^b) &\geq m(P_{a-1}\cup U_{n-a-1}^b,2)-2\\
&= m(P_{a-1},2)+m(U_{n-a-1}^b,2)+(a-2)(n-a-1)-2\\
&\geq m(P_{a-1},2)+(a-2)(n-a-1)\\
&\geq \frac{(a-3)(a-4)}{2}+(a-2)b\geq 19,\\
b_3(P_{a-1}\cup U_{n-a-1}^b) &\geq m(P_{a-1}\cup U_{n-a-1}^b,3)-2(n-b-4)\\
&= m(P_{a-1},3)+(n-a-1)m(P_{a-1},2)\\
&\quad +(a-2)m(U_{n-a-1}^b,2)+m(U_{n-a-1}^b,3)-2(n-b-4)\\
&\geq (n-a-1)m(P_{a-1},2)+(n-b-4)m(C_b,2)\\
&\quad -2(n-b-4)\\
&\geq (n-a-1)m(P_{a-1},2)\geq \frac{b(a-3)(a-4)}{2}\geq 12.
\end{aligned}$$

Therefore $b_k(G) \geq b_k(B_n^4)$ for $k = 2, 3, 4$, and it is strict for $k = 3$.

Case 2. $\widehat{G} \neq G$.

Let G_0 be the graph obtained by attaching a pendent vertex to the pendent vertex of B_{11}^4. Note that

$$b_2(G_0) = 58, \quad b_3(G_0) = 109, \quad b_4(G_0) = 85,$$
$$b_2(B_{12}^4) = 55, \quad b_3(B_{12}^4) = 89, \quad b_4(B_{12}^4) = 46.$$

If $G = G_0$, then the result follows.

Suppose that $G \neq G_0$. Then we can choose a pendent vertex u, being adjacent to v, in G such that $G - u \neq B_{n-1}^4$. By Lemma 1 (i),

$$b_k(G) = b_k(G - u) + b_{k-1}(G - u - v).$$

By the induction hypothesis, we have $b_k(G - u) \geq b_k(B_{n-1}^4)$ for $k = 2, 3, 4$, and it is strict for $k = 3$. So it suffices to show that $b_{k-1}(G - u - v) \geq b_{k-1}(P_5 \cup C_4)$ for $k = 2, 3, 4$.

Subcase 2.1. $G - u - v$ contains $\widehat{G}$. By Lemma 2, $b_{k-1}(G - u - v) \geq b_{k-1}(C_a \cup C_b)$. By Sachs theorem,

$$\begin{aligned}
b_1(G - u - v) &\geq m(C_a \cup C_b, 1) = a + b > 8, \\
b_2(G - u - v) &\geq b_2(C_a \cup C_b) \geq m(C_a \cup C_b, 2) - 2 \geq ab > 19, \\
b_3(G - u - v) &\geq b_3(C_a \cup C_b) \geq m(C_a \cup C_b, 3) - 2a \\
&= m(C_a, 3) + bm(C_a, 2) + am(C_b, 2) + m(C_b, 3) - 2a \\
&\geq bm(C_a, 2) = \frac{a(a-3)b}{2} > 12.
\end{aligned}$$

Subcase 2.2. $G - u - v$ contains exactly one cycle C_r, $r \in \{a, b\}$. If $r = 4$, then $P_5 \cup C_4$ is a subgraph of $G - u - v$, and by Lemma 2, $b_{k-1}(G - u - v) \geq b_{k-1}(P_5 \cup C_4)$ for $k = 2, 3, 4$. Suppose that $r \geq 6$. Then $G - u - v$ contains $C_r \cup P_{s-1}$ where $\{r, s\} = \{a, b\}$. By Lemma 2 and Sachs theorem,

$$\begin{aligned}
b_1(G - u - v) &\geq b_1(C_r \cup P_{s-1}) = r + s - 2 = a + b - 2 \geq 8, \\
b_2(G - u - v) &\geq b_2(C_r \cup P_{s-1}) \geq m(C_r, 2) + r(s - 2) \\
&= \frac{r(r-3)}{2} + r(s-2) \geq 19, \\
b_3(G - u - v) &\geq b_3(C_r \cup P_{s-1}) \geq m(C_r \cup P_{s-1}, 3) \\
&\geq m(C_r, 2)(s-2) = \frac{r(r-3)}{2}(s-2) \geq 12.
\end{aligned}$$

Combining Subcases 2.1 and 2.2, $b_{k-1}(G - u - v) \geq b_{k-1}(P_5 \cup C_4)$ for $k = 2, 3, 4$. Therefore $b_k(G) \geq b_k(B_n^4)$ for $k = 2, 3, 4$, and it is strict for $k = 3$. Now the result follows. $\square$

Using the increasing property (2) of energy, and Theorems 1, 2 and 3, we have

Theorem 4. *Let $G \in B(n)$.*
(i) if $G \in B_\theta(n)$ and $G \neq B_n^1, B_n^2$, where $n \geq 8$, then $E(G) > E(B_n^2)$;
(ii) if $G \in B_{\infty_1}(n)$ and $G \neq B_n^3$, where $n \geq 10$, then $E(G) > E(B_n^3)$;
(iii) if $G \in B_{\infty_2}(n)$ and $G \neq B_n^4$, where $n \geq 11$, then $E(G) > E(B_n^4)$.

We list the b_k-values, $k \geq 2$, for B_n^4, B_n^3 and B_n^2 in Table 1, from which we have

Lemma 7. *$B_9^3 \succ B_9^2$ and $B_n^4 \succ B_n^3 \succ B_n^2$ for $n \geq 10$.*

G	$b_2(G)$	$b_3(G)$	$b_4(G)$	$b_k(G)$ for $k \geq 4$
B_n^4	$8n-41$	$19n-139$	$12n-98$	0
B_n^3	$6n-25$	$11n-71$	$6n-46$	0
B_n^2	$4n-17$	$3n-17$	0	0

Table 1. b_k-values, $k \geq 2$, for graphs B_n^4, B_n^3 and B_n^2.

Let $G \in B(n)$ and $G \neq B_n^1$, B_n^2, where $n \geq 8$. By Lemma 7 and Theorems 1, 2 and 3, we have $G \succ B_n^2$. Thus we have

Theorem 5. *If $G \in B(n)$ and $G \neq B_n^1, B_n^2$, where $n \geq 8$, then $E(G) > E(B_n^2)$.*

Remark. By direct calculation, we find $E(B_n^1) < E(B_n^2)$ for $7 \leq n \leq 20$. However, for $n \geq 7$,

$$b_2(B_n^1) = 5n-23 > 4n-17 = b_2(B_n^2), \quad b_3(B_n^1) = 2n-11 < 3n-17 = b_3(B_n^2),$$

and so the relation "$\succ$" cannot be used to order B_n^1 and B_n^2.

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