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Note

Minimal Spectrum-Sums of Bipartite Graphs with Exactly Two Vertex-Disjoint Cycles

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The spectrum-sum of a graph is defined as the sum of the absolute values of its eigenvalues. The graphs with minimal spectrum-sums in the class of connected bipartite graphs with exactly two vertex-disjoint cycles, in the class of connected bipartite graphs with exactly two vertex-disjoint cycles whose lengths are congruent with 2 modulo 4, and in the class of connected bipartite graphs with exactly two vertex-disjoint cycles one of which has length congruent with 2 modulo 4, are determined, respectively.

INTRODUCTION

Let G be a simple graph with n vertices.[1] The characteristic polynomial of G is the characteristic polynomial of its adjacency matrix, denoted by $\phi(G, \lambda)$.[2,3] The eigenvalues of G denoted by $\lambda_1, \ldots, \lambda_n$, are the roots of $\phi(G, \lambda) = 0$. The set of graph-eigenvalues is also called the spectrum of the graph.[4] The spectrum-sum of G is defined as the sum of the absolute values of all elements in the graph-spectrum:

$$E(G) = |\lambda_1| + |\lambda_2| + \ldots + |\lambda_n| .$$

In the literature, the energy of a graph is usually employed for the spectrum-sum, *e.g.*, Refs. 5–8. This term was introduced by Gutman[9] and an explanation why he had chosen this term is given in Ref. 10. We choose the term spectrum-sum since in physical sciences energy represents a measurable quantity.

If G is the molecular graph of a conjugated hydrocarbon, often called the Hückel graph,[11] then the corresponding set of eigenvalues is called the Hückel spectrum.[12] The connection between the graph spectrum and Hückel spectrum and the role of Hückel spectrum in the theory of conjugated molecules were discussed in detail elsewhere.[13,14] The use of the Hückel spectrum in chemistry has been recently presented, for example, in this journal.[15]

For a bipartite graph G (depicting the alternant structures)[16] with n vertices, its characteristic polynomial can be written as:

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

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where $b_k(\mathrm{G}) \geq 0$ for $k = 0,1,...,\left\lfloor \frac{n}{2} \right\rfloor$. For convenience, let $b_k(\mathrm{G}) = 0$ for $k < 0$ or $k > \left\lfloor \frac{n}{2} \right\rfloor$. We also note that the spectrum-sum can be calculated by the Coulson integral formula:[17]

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

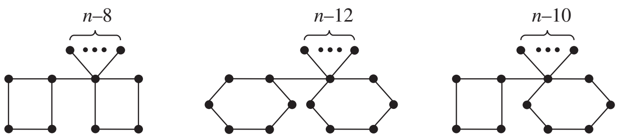
Thus, one can define a quasi-order relation over the class of all bipartite graphs: if G and G' are bipartite graphs with n vertices, then:

$$\mathrm{G} \succeq \mathrm{G}' \Leftrightarrow b_k(\mathrm{G}) \geq b_k(\mathrm{G}') \text{ for } k = 0,1,...,\left\lfloor \frac{n}{2} \right\rfloor.$$

If $\mathrm{G} \succeq \mathrm{G}'$ and there is a k_0 such that $b_{k_0}(\mathrm{G}) > b_{k_0}(\mathrm{G}')$, then we write $\mathrm{G} \succ \mathrm{G}'$. According to the Coulson integral formula for energy, for bipartite graphs G and G', we have:

$$\mathrm{G} \succ \mathrm{G}' \Rightarrow \mathrm{E(G)} > \mathrm{E(G')} \quad (1)$$

Gutman[18] determined acyclic conjugated structures (trees) with extremal Hückel π-electron energies (spectrum-sums). That work triggered interest in determining graphs with minimal or maximal spectrum sums.[5–8,19–26] In the present report, we join these efforts by studying graphs with minimal spectrum-sums in the class of bipartite graphs with exactly two vertex-disjoint cycles. Examples of these graphs are shown in Figure 1.



$\mathrm{B}^{4,4}_{4,n-4}$ $\mathrm{B}^{6,6}_{6,n-6}$ $\mathrm{B}^{4,6}_{4,n-4}$

Figure 1. Examples of graphs with minimal spectrum-sums in the class of bipartite graphs with exactly two vertex-disjoint cycles.

PRELIMINARIES

Let P_n and C_n be the path and cycle with n vertices, respectively. Let U^l_n be the graph obtained by attaching $n–l$ pendent vertices to a vertex of the cycle C_l. The vertex-disjoint union of graphs G and H is denoted by $\mathrm{G} \cup \mathrm{H}$, $[p]$G denotes the vertex-disjoint union of p copies of G.

Lemma 1.[10] – Let G be a bipartite graph and let uv be a bridge of G. Then:

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

According to Lemma 1, it is easy to see that the following two lemmas hold.

Lemma 2. – Let G be a bipartite graph and let uv be a bridge of G. Then $\mathrm{G} \succ \mathrm{G} - uv$.

For example, if an acyclic graph G with n vertices contains a subgraph H with $t < n$ vertices, then according to Lemma 2, we have $\mathrm{G} \succ \mathrm{H} \cup [n-t]\mathrm{P}_1$.

Lemma 3. – Let G and G' be two bipartite graphs with n vertices. Let uv be a bridge of G and $u'v'$ be a bridge of G'. If $\mathrm{G} - uv \succeq \mathrm{G}' - u'v'$ and $\mathrm{G} - u - v \succ \mathrm{G}' - u' - v'$, or $\mathrm{G} - uv \succ \mathrm{G}' - u'v'$ and $\mathrm{G} - u - v \succeq \mathrm{G}' - u' - v'$ then $\mathrm{G} \succ \mathrm{G}'$.

According to Theorems 4 and 5 in Ref. 5 and Theorem 4 in Ref. 6, we have:

Lemma 4.[5,6] – Let G be an n-vertex bipartite unicyclic graph whose unique cycle length is l. If $\mathrm{G} \neq \mathrm{U}^l_n$, then $\mathrm{G} \succ \mathrm{U}^l_n$. If $l > 4$ then $\mathrm{U}^l_n \succ \mathrm{U}^4_n$. If $l > 6$ then $\mathrm{U}^l_n \succ \mathrm{U}^6_n$.

Lemma 5.[26] – Let G_1 and G_2 be two vertex-disjoint bipartite graphs. Then for any k ≥ 0,

$$b_k(\mathrm{G}_1 \cup \mathrm{G}_2) = \sum_{i=0}^{k} b_i(\mathrm{G}_1) b_{k-i}(\mathrm{G}_2).$$

Proof: Let $n_i = |\mathrm{V}(\mathrm{G}_i)|$ for i = 1,2. Note that:

$$\sum_{i=0}^{\lfloor n/2 \rfloor} (-1)^k b_k(\mathrm{G}_1 \cup \mathrm{G}_2) x^{n-2k} =$$
$$\phi(\mathrm{G}_1 \cup \mathrm{G}_2, x) =$$
$$\phi(\mathrm{G}_1, x)\,\phi(\mathrm{G}_2, x) =$$
$$\sum_{i=0}^{\lfloor n_1/2 \rfloor} (-1)^i b_i(\mathrm{G}_1) x^{n_1-2i} \sum_{i=0}^{\lfloor n_2/2 \rfloor} (-1)^i b_i(\mathrm{G}_2) x^{n_2-2i}.$$

The result follows directly. □

RESULTS

Let $\mathrm{B}^{l_1,l_2}_{n_1,n_2}$ be the graph obtained by adding an edge between the vertex of maximal degree in $\mathrm{U}^{l_1}_{n_1}$ and the vertex of maximal degree in $\mathrm{U}^{l_2}_{n_2}$. Let G be an n-vertex connected bipartite graph with exactly two vertex-disjoint cycles. Then there are two vertex-disjoint cycles $\mathrm{C}^{(1)}$ and $\mathrm{C}^{(2)}$ in G with lengths l_1 and l_2, respectively, and there is a unique path P connecting a vertex say $u = u_1$ in $\mathrm{C}^{(1)}$ and a vertex say v in $\mathrm{C}^{(2)}$, such that each edge in P is a bridge of G, where l_1 and l_2 are even and at least four. Let u_2 be the unique neighbor of u_1 in P. Then G– u_1u_2 consists of two components G_1 containing the cycle $\mathrm{C}^{(1)}$ and G_2 containing the cycle $\mathrm{C}^{(2)}$. Let $n_i = |\mathrm{V}(\mathrm{G}_i)|$, i = 1,2 Obviously, $n_1 + n_2 = n$.

Theorem 6. – Let G be an n-vertex connected bipartite graph with exactly two vertex-disjoint cycles, where n ≥ 9. If $\mathrm{G} \neq \mathrm{B}^{4,4}_{4,n-4}$ then $\mathrm{G} \succ \mathrm{B}^{4,4}_{4,n-4}$.

Proof: According to Lemma 4, $G_i \succeq U_{n_i}^4$ for i = 1,2. According to Lemma 5:

$$G - u_1u_2 = G_1 \cup G_2 \succeq U_{n_1}^4 \cup U_{n_2}^4 .$$

Now we consider the graph $G - u_1 - u_2 = (G_1 - u_1) \cup (G_2 - u_2)$. Note that $G_1 - u_1$ is an acyclic graph containing a path P_3. According to Lemma 2, $G_1 - u_1 \succeq P_3[n_1 - 4]P_1$, and if u_2 lies on the cycle $C^{(2)}$, then $G_2 - u_2 \succeq P_3 \cup [n_2 - 4]P_1$. Suppose that u_2 lies outside the cycle $C^{(2)}$. According to Lemma 2, $G_2 - u_2 \succeq C_{l_2} \cup [n_2 - 1 - l_2]P_1$. It is easily seen that:

$$b_1(C_{l_2} \cup [n_2 - 1 - l_2]P_1) = l_2 > 2 = b_1(P_3 \cup [n_2 - 4]P_1),$$

and $b_k(C_{l_2} \cup [n_2 - 1 - l_2]P_1) \geq 0 = b_k(P_3 \cup [n_2 - 4]P_1)$ for all $k \geq 2$. Thus, we have $G_2 - u_2 \succeq C_{l_2} \cup [n_2 - 1 - l_2]P_1 \succ P_3 \cup [n_2 - 4]P_1$. It follows that $G_2 - u_2 \succeq P_3 \cup [n_2 - 4]P_1$ whether u_2 lies on the cycle $C^{(2)}$ or not. Thus we have proved that: $G_1 - u_1 \succeq P_3 \cup [n_1 - 4]P_1$ and $G_2 - u_2 \succeq P_3 \cup [n_2 - 4]P_1$. Now according to Lemma 5:

$$G - u_1 - u_2 = (G_1 - u_1) \cup (G_2 - u_2) \succeq [2]P_3 \cup [n - 8]P_1.$$

If $\min\{n_1,n_2\} = 4$ say $n_1 = 4$ then since $G \neq B_{4,n-4}^{4,4}$ we have $G_2 - u_2$ containing the path or the star on four vertices as a subgraph, and so $b_1(G - u_1 - u_2) = b_1(G_1 - u_1) + b_1(G_2 - u_2) \geq 2 + 3 > 4 = b_1([2]P_3 \cup [n - 8]P_1)$, implying:

$$G - u_1 - u_2 = (G_1 - u_1) \cup (G_2 - u_2) \succ [2]P_3 \cup [n - 8]P_1.$$

According to Lemma 3, we have $G \succ B_{n_1,n_2}^{4,4}$ and if $\min\{n_1, n_2\} = 4$, then $G \succ B_{n_1,n_2}^{4,4} = B_{4,n-4}^{4,4}$ and so the result follows. By direct calculation:

$$\begin{aligned}\phi(U_{n_1}^4 \cup U_{n_2}^4, \lambda) = {} & [\lambda^{n_1} - n_1\lambda^{n_1-2} + (2n_1 - 8)\lambda^{n_1-4}] \times \\ & [\lambda^{n_2} - n_2\lambda^{n_2-2} + (2n_2 - 8)\lambda^{n_2-4}] = \\ & [\lambda^n - n\lambda^{n-2} + (n_1n_2 + 2n - 16)\lambda^{n-4} - \\ & 4(n_1n_2 - 2n)\lambda^{n-6} + \\ & 4(n_1n_2 - 4n + 16)\lambda^{n-8}.\end{aligned}$$

Suppose that $\min\{n_1,n_2\} > 4$. Then $n_1n_2 > 4(n - 4)$. Thus $b_2(U_{n_1}^4 \cup U_{n_2}^4) = n_1n_2 + 2n - 16 > 4(n - 4) + 2n - 16 \geq b_2(U_4^4 \cup U_{n-4}^4)$. Similarly, $b_k(U_{n_1}^4 \cup U_{n_2}^4) > b_k(U_4^4 \cup U_{n-4}^4)$ for k = 3,4 Note that $b_k(U_{n_1}^4 \cup U_{n_2}^4) = b_k(U_4^4 \cup U_{n-4}^4) = 0$ for $k \geq 4$. It follows that $U_{n_1}^4 \cup U_{n_2}^4 \succ U_4^4 \cup U_{n-4}^4$. According to Lemma 3, $B_{n_1,n_2}^{4,4} \succ B_{4,n-4}^{4,4}$. It follows that $G \succeq B_{n_1,n_2}^{4,4} \succ B_{4,n-4}^{4,4}$. □

Theorem 7. – Let G be an n-vertex connected bipartite graph with exactly two vertex-disjoint cycles, where $n \geq 13$. If both cycle lengths of G are congruent with 2 modulo 4 and $G \neq B_{6,n-6}^{6,6}$, then $G \succ B_{6,n-6}^{6,6}$.

Proof: According to Lemma 4, $G_i \succeq U_{n_i}^6$ for i = 1,2. According to Lemma 5, $G - u_1u_2 = G_1 \cup G_2 \succeq U_{n_1}^6 \cup U_{n_2}^6$.

Now we consider the graph $G - u_1 - u_2 = (G_1 - u_1) \cup (G_2 - u_2)$. According to Lemma 2, $G_1 - u_1 \succeq P_5 \cup [n_1 - 6]P_1$, and if u_2 lies on the cycle $C^{(2)}$ then $G_2 - u_2 \succeq P_5 \cup [n_2 - 6]P_1$.

Suppose that u_2 lies outside the cycle $C^{(2)}$. According to Lemma 2, $G_2 - u_2 \succeq C_{l_2} \cup [n_2 - 1 - l_2]P_1$. It is easily seen that:

$$b_1(C_{l_2} \cup [n_2 - 1 - l_2]P_1) = l_2 > 4 = b_1(P_5 \cup [n_2 - 6]P_1),$$

$$b_2(C_{l_2} \cup [n_2 - 1 - l_2]P_1) = \frac{l_2(l_2 - 3)}{2} > 3 = b_2(P_5 \cup [n_2 - 6]P_1),$$

and $b_k(C_{l_2} \cup [n_2 - 1 - l_2]P_1) \geq 0 = b_k(P_5 \cup [n_2 - 6]P_1)$ for all $k \geq 3$. Thus, we have $G_2 - u_2 \succeq C_{l_2} \cup [n_2 - 1 - l_2]P_1 \succ P_5 \cup [n_2 - 6]P_1$. It follows that $G_2 - u_2 \succeq P_5 \cup [n_2 - 6]P_1$ whether u_2 lies on the cycle $C^{(2)}$ or not. According to Lemma 5:

$$G - u_1 - u_2 = (G_1 - u_1) \cup (G_2 - u_2) \succeq [2]P_5 \cup [n - 12]P_1.$$

If $\min\{n_1,n_2\} = 6$ say $n_1 = 6$, then since $G \neq B_{6,n-6}^{6,6}$ we have $G_2 - u_2$ containing a subgraph formed by attaching a pendent vertex to the path P_5, and so $b_1(G - u_1 - u_2) = b_1(G_1 - u_1) + b_1(G_2 - u_2) \geq 4 + 5 > 8 = b_1([2]P_5 \cup [n - 12]P_1$, implying:

$$G - u_1 - u_2 = (G_1 - u_1) \cup (G_2 - u_2) \succ [2]P_5 \cup [n - 12]P_1.$$

According to Lemma 3, we have $G \succeq B_{n_1,n_2}^{6,6}$, and if $n_1 = 6$, then $G \succ B_{n_1,n_2}^{6,6} = B_{6,n-6}^{6,6}$, and so the result follows. By direct calculation:

$$\begin{aligned}\phi(U_{n_1}^6 \cup U_{n_2}^6, \lambda) = {} & \\ & [\lambda^{n_1} - n_1\lambda^{n_1-2} + (4n_1 - 5)\lambda^{n_1-4} - (3n_1 - 18)\lambda^{n_1-6}] \times \\ & [\lambda^{n_2} - n_2\lambda^{n_2-2} + (4n_2 - 5)\lambda^{n_2-4} - (3n_2 - 18)\lambda^{n_2-6}] = \\ & \lambda^n - n\lambda^{n-2} + (n_1n_2 + 4n - 30)\lambda^{n-4} - \\ & (8n_1n_2 - 12n - 36)\lambda^{n-6} + (22n_1n_2 - 78n + 225)\lambda^{n-8} - \\ & (24n_1n_2 - 117n + 540)\lambda^{n-10} + (9n_1n_2 - 54n - 324)\lambda^{n-12}.\end{aligned}$$

If $\min\{n_1,n_2\} > 6$ then $n_1,n_2 > 6(n - 6)$, and from the characteristic polynomial above, we have $U_{n_1}^6 \cup U_{n_2}^6 \succ U_6^6 \cup U_{n-6}^6$. According to Lemma 3, we have $G \succeq B_{n_1,n_2}^{6,6} = B_{6,n-6}^{6,6}$. □

The following theorem was reported in Ref. 26. Here we give an alternate proof.

Theorem 8. – Let G be an n-vertex connected bipartite graph with exactly two vertex-disjoint cycles, where $n \geq 11$. If one cycle length of G is congruent with 2 modulo 4 and $G \neq B_{4,n-4}^{4,6}$, then $G \succ B_{4,n-4}^{4,6}$.

Proof: Suppose without loss of generality that $l_2 \equiv 2$ (mod 4). According to Lemma 4, $G_1 \succeq U^4_{n_1}$ and $G_2 \succeq U^6_{n_2}$. According to Lemma 5, $G - u_1u_2 = G_1 \cup G_2 \succeq U^4_{n_1} \cup U^6_{n_2}$.

Now we consider the graph $G - u_1 - u_2 = (G_1 - u_1) \cup (G_2 - u_2)$. According to Lemma 2, $G_1 - u_1 \succeq P_3 \cup [n_1 - 4] P_1$, and if u_2 lies on the cycle $C^{(2)}$, then $G_2 - u_2 \succeq P_5 \cup [n_2 - 6]P_1$.

Suppose that u_2 lies outside the cycle $C^{(2)}$. According to Lemma 2, $G_2 - u_2 \succeq C_{l_2} \cup [n_2 - 1 - l_2] P_1$. It is easily seen that:

$$b_1(C_{l_2} \cup [n_2-1-l_2]P_1) = l_2 > 4 = b_1(P_5 \cup [n_2 - 6]P_1),$$

$$b_2(C_{l_2} \cup [n_2-1-l_2]P_1) = \frac{l_2(l_2-3)}{2} > 3 = b_2(P_5 \cup [n_2-6]P_1),$$

and $b_k(C_{l_2} \cup [n_2 - 1 - l_2]P_1) \geq 0 = b_k(P_5 \cup [n_2 - 6]P_1)$ for all $k \geq 3$. Thus, we have $G_2 - u_2 \succeq C_{l_2} \cup [n_2 - 1 - l_2]P_1 \succ P_5 \cup [n_2 - 6]P_1$. It follows that $G_2 - u_2 \succeq P_5 \cup [n_2 - 6]P_1$ whether u_2 lies either on the cycle $C^{(2)}$ or not. According to Lemma 5:

$$G - u_1 - u_2 = (G_1 - u_1) \cup (G_2 - u_2) \succeq P_3 \cup P_5 \cup [n - 10]P_1.$$

If $n_1 = 4$ then since, $G \neq B^{4,6}_{4,n-4}$, we have $G_2 - u_2$ containing a subgraph formed by attaching a pendent vertex to the path P_5 and so $b_1(G - u_1 - u_2) = b_1(G_1 - u_1) + b_1(G_2 - u_2) \geq 2 + 5 > 6 = b_1(P_3 \cup P_5 \cup [n - 10]P_1$, implying:

$$G - u_1 - u_2 = (G_1 - u_1) \cup (G_2 - u_2) \succ P_3 \cup P_5 [n - 10] P_1.$$

According to Lemma 3, we have $G \succeq B^{4,6}_{n_1,n_2}$, and if $n_1 = 4$, then $G \succ B^{4,6}_{n_1,n_2} = B^{4,6}_{4,n-4}$, and so the result follows. By direct calculation:

$$\phi(U^4_{n_1} \cup U^6_{n_2}, \lambda) = \lambda^n - n\lambda^{n-2} + (n_1n_2+2n_2+2n-23)\lambda^{n-4} - (6n_1n_2 + 10n_2 - 15n - 18)\lambda^{n-6} + (11n_1n_2 + 16n_2 - 48n + 120)\lambda^{n-8} - (6n_1n_2 + 12n_2 - 36n + 144)\lambda^{n-10}.$$

If $n_1 > 4$ then $f(n_1,n_2) = an_1n_2 + bn_2 > f(4, n-4)$ for $(a,b) = (1,2)$, $(6,10)$, $(11,16)$, $(6,12)$ and thus from the characteristic polynomial above, we have $U^4_{n_1} \cup U^6_{n_2} \cup U^4_4 \cup U^6_{n-4}$. According to Lemma 3, we have $G \succeq B^{4,6}_{n_1,n_2} \succ B^{4,6}_{4,n-6}$. □

Let G be an n-vertex connected bipartite graph with exactly two vertex-disjoint cycles, where $n \geq 9$. According to Theorems 6, 7 and 8, and using (1), we have:

(i) If $G \neq B^{4,4}_{4,n-4}$ then $E(G) > E(B^{4,4}_{4,n-4})$.

(ii) If both cycle lengths of G are congruent with 2 modulo 4 and $G \neq B^{6,6}_{6,n-6}$ where $n \geq 13$ then $E(G) > E(B^{6,6}_{6,n-6})$

(iii) If one cycle length of G is congruent with 2 modulo 4 and $G \neq B^{4,6}_{4,n-4}$, where $n \geq 11$ then $E(G) > E(B^{4,6}_{4,n-4})$.

For the graphs $B^{4,4}_{4,n-4}$, $B^{4,6}_{4,n-4}$ and $B^{6,6}_{6,n-6}$ with $n \geq 12$, it may be easily checked by Lemmas 3 and 4 or by the characteristic polynomials that $E(B^{4,4}_{4,n-4}) < E(B^{4,6}_{4,n-4}) < E(B^{6,6}_{6,n-6})$.

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SAŽETAK

Minimalne spektralne sume bipartitnih grafova s točno dva prstena razmaknuta jednim bridom

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Spektralna suma grafa definirana kao zbroj apsolutnih vrijednosti svih elemenata u spektru grafa. Pronađeni su grafovi s minimalnim spektralnim sumama u klasi bipartitnih grafova s točno dva prstena razmaknuta jednim bridom gdje su veličine prstenova sukladno s 2 modulo 4 i u klasi bipartitnih grafova s točno dva prstena razmaknuta jednim bridom gdje je veličina jednoga prstena sukladana s 2 modulo 4.