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On the Path Energy of Bicyclic Graphs

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Abstract

Let G be a graph with the vertex set $\{v_1, \ldots, v_n\}$. The path matrix $P(G)$ is an $n \times n$ matrix whose (i, j)-entry is the maximum number of internally disjoint v_iv_j-paths in G, if $i \neq j$, and zero otherwise. The sum of absolute values of the eigenvalues of $P(G)$ is called the path energy of G. In this paper the path energy of bicyclic graphs are investigated. In particular, among bicyclic graphs of a fixed order, the graphs with maximum and minimum path energy are characterized. Using these results, we provide affirmative answers to some conjectures proposed in *MATCH Commun. Math. Comput. Chem.* **79** (2018) 387–398.

1 Introduction

Throughout this paper, all graphs are simple, that is, with no loops and multiple edges. Let G be a graph of order n with the vertex set $V(G) = \{v_1, \ldots, v_n\}$. In [6], the *path matrix* of graph G is defined as an $n \times n$ matrix $P(G)$ whose (i, j)-entry is the maximum number of internally disjoint paths between the vertices v_i and v_j, when $i \neq j$ and is zero when $i = j$. The *energy* of a graph G, $E(G)$, is defined to be the sum of absolute values of eigenvalues of adjacency matrix of G, see [3]. Similarly, the *path energy* of G,

$PE(G)$, is defined as the sum of absolute values of eigenvalues of $P(G)$. Since $P(G)$ is a real symmetric matrix, its eigenvalues are real. The all-one column vector and all-one matrix are denoted by j and J , respectively. Also J_n denotes the all-one $n \times n$ matrix. Let G be a graph. Denote by $pr(G)$ the graph obtained by removing all pendant vertices of G. If $pr(G)$ still contains pendent vertices, then repeat this operation as many times as necessary until the resulting graph, $pr^*(G)$, is free of pendent vertices. As in [5], there are three types of bicyclic graphs without pendent vertices which are shown in Figure 1. In $\mathcal{B}^{(1)}(a,b)$ and $\mathcal{B}^{(2)}(a,b)$, we assume that $a,b \geq 3$ and in $\mathcal{B}^{(3)}(a,b,c)$, $a,b \geq c+3$.

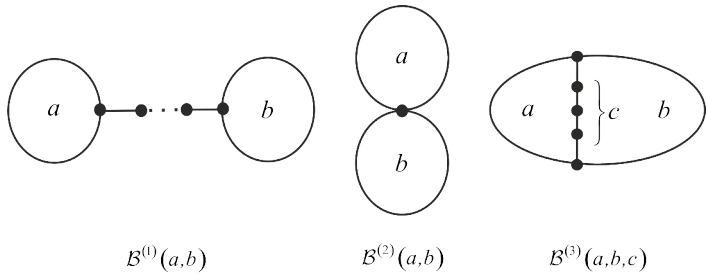

Figure 1. The types of bicyclic graphs.

For $i = 1, 2, 3$, we say that a graph G is a bicyclic graph of Type $\mathcal{B}^{(i)}$, if $pr^*(G) \in \mathcal{B}^{(i)}$. we denote by $\mathcal{B}_n$ the set of all bicyclic graphs of order n. In [1], the path energy of unicyclic graphs are determined. Also in [5] the following conjectures were proposed for the bicyclic graphs.

Conjecture 1. *If $G \in \mathcal{B}_n$, then $PE(G)$ is maximal if and only if $G \in \mathcal{B}^{(3)}$, for $n = a+b-c-2$, $a,b \geq 3$, $c \geq 0$.*

Conjecture 2. *If $G \in \mathcal{B}_n$, then $PE(G)$ is minimal if and only if $pr^*(G) \cong \mathcal{B}^{(2)}(3,3)$.*

Motivated by these conjectures, in Section 2 we obtain some lower and upper bounds on the path energy of bicyclic graphs. Using these bounds, in Section 3 we prove the validity of Conjectures 1 and 2.

2 Path Energy of Bicyclic Graphs

In this section, we investigate the path energy of bicyclic graphs. To do this, we need the following theorem.

Theorem 1. *Let A be a matrix as follows:*

$$A = \begin{pmatrix} p_{11}(J-I) & p_{12}J & \cdots & p_{1k}J \\ p_{21}J & p_{22}(J-I) & \cdots & p_{2k}J \\ \vdots & \vdots & \ddots & \vdots \\ p_{k1}J & p_{k2}J & \cdots & p_{kk}(J-I) \end{pmatrix},$$

such that the (i,j) block of A is an $n_i \times n_j$ matrix. Then

$$\det(xI - A) = (x + p_{11})^{n_1 - 1} \cdots (x + p_{kk})^{n_k - 1} \det(xI - B),$$

where

$$B = \begin{pmatrix} p_{11}(n_1 - 1) & p_{12}n_2 & \cdots & p_{1k}n_k \\ p_{21}n_1 & p_{22}(n_2 - 1) & \cdots & p_{2k}n_k \\ \vdots & \vdots & \ddots & \vdots \\ p_{k1}n_1 & p_{k2}n_2 & \cdots & p_{kk}(n_k - 1) \end{pmatrix}.$$

Proof. For every positive integer m, let M_m be an $m \times (m-1)$ matrix defined as:

$$M_m = \begin{pmatrix} j_{m-1}^T \\ -I_{m-1} \end{pmatrix}.$$

Now, define the $n \times k$ matrix C and $n \times (n-k)$ matrix D by:

$$C = \begin{pmatrix} j_{n_1} & & 0 \\ & \ddots & \\ 0 & & j_{n_k} \end{pmatrix} \qquad D = \begin{pmatrix} M_{n_1} & & 0 \\ & \ddots & \\ 0 & & M_{n_k} \end{pmatrix}$$

It is not hard to see that $AC = CB$. Also, if

$$E = \begin{pmatrix} -p_{11}I_{n_1-1} & & 0 \\ & \ddots & \\ 0 & & -p_{kk}I_{n_k-1} \end{pmatrix},$$

then $AD = DE$. Now, define $U = \left(\begin{array}{c|c} C & D \end{array} \right)$. It can be seen that U is an $n \times n$ matrix and the columns of U are independent. Therefore U is invertible. Also,

$$AU = \left(\begin{array}{c|c} AC & AD \end{array} \right) = \left(\begin{array}{c|c} CB & DE \end{array} \right) = U \begin{pmatrix} B & 0 \\ 0 & E \end{pmatrix},$$

which gives $U^{-1}AU = \begin{pmatrix} B & 0 \\ 0 & E \end{pmatrix}$. Therefore $\det(xI - A) = \det(xI - B)\det(xI - E)$, and this completes the proof. ■

A *multilinear polynomial* with variables $x_1, \ldots, x_n$ is a polynomial whose monomials are of the form $x_{i_1} \cdots x_{i_k}$, where $1 \leq i_1 < i_2 < \cdots < i_k \leq n$.

Lemma 2. *Let $p(x_1, \ldots, x_n)$ be a multilinear polynomial. For every $r_1, \ldots, r_n \in \{0, 1\}$ define:*

$$S_p(r_1, \ldots, r_n) = (-1)^{\sum r_i} \sum (-1)^{\sum t_i} p(t_1, \ldots, t_n),$$

where the summation is over all $t_1, \ldots, t_n \in \{0, 1\}$ such that $0 \leq t_i \leq r_i$, $i = 1, \ldots, n$. Suppose that for all $r_1, \ldots, r_n \in \{0, 1\}$, $S_p(r_1, \ldots, r_n) \geq 0$. Then, for all $c_1, \ldots, c_n \geq 0$, $p(c_1, \ldots, c_n) \geq 0$.

Proof. We apply induction on n. Let $n = 1$. Since $p(x_1) = ax_1 + b$, by assumption we have $b = p(0) \geq 0$ and $a = p(1) - p(0) \geq 0$. Thus, for $t \geq 0$, $p(t) \geq 0$. Now, suppose that the result holds for $n - 1$ ($n \geq 2$) and p is a multilinear polynomial with n variables that satisfies the assumption of lemma. Let

$$g(x_1, \ldots, x_{n-1}) = p(x_1, \ldots, x_{n-1}, 0),$$
$$h(x_1, \ldots, x_{n-1}) = p(x_1, \ldots, x_{n-1}, 1) - p(x_1, \ldots, x_{n-1}, 0).$$

Since p is multilinear, $\frac{\partial p}{\partial x_n} = h$. Let $r_1, \ldots, r_{n-1} \in \{0, 1\}$. One can see that:

$$S_g(r_1, \ldots, r_{n-1}) = S_p(r_1, \ldots, r_{n-1}, 0) \geq 0,$$
$$S_h(r_1, \ldots, r_{n-1}) = S_p(r_1, \ldots, r_{n-1}, 1) \geq 0.$$

So by induction hypothesis, for all $c_1, \ldots, c_{n-1} \geq 0$, $g(c_1, \ldots, c_{n-1}) \geq 0$ and $h(c_1, \ldots, c_{n-1}) \geq 0$. This implies that $p(c_1, \ldots, c_n)$ is an increasing function of c_n and $p(c_1, \ldots, c_{n-1}, 0) \geq 0$. So $p(c_1, \ldots, c_n) \geq 0$. ■

Lemma 2 allows us to prove some inequalities between multilinear polynomials by computing a finite number of summations. All computations in this paper were done using the Sage Mathematics Software System [4]. Now, we are in a position to investigate the path energy of bicyclic graphs.

2.1 Bicyclic Graphs of Type $\mathcal{B}^{(1)}$

In this subsection, we study the path energy of the first type of bicyclic graphs.

Theorem 3. *Let $a, b \geq 3$ and G be a bicyclic graph of Type $\mathcal{B}^{(1)}(a, b)$ of order $n = a+b+c$.*

(i) If $c = 0$, then $PE(G) = 4n - 8$.

(ii) If $c > 0$, then $|PE(G) - (4n - 2c - 9)| \leq 1$.

Proof. (i) Let $v_1, \ldots, v_a$ be the vertices of the cycle of length a, and $v_{a+1}, \ldots, v_{a+b}$ be the vertices of the cycle of length b. The path matrix of G in this ordering is as follows:

$$P(G) = \begin{pmatrix} 2(J_a - I) & J \\ J & 2(J_b - I) \end{pmatrix}.$$

Now, by Theorem 1 the characteristic polynomial of $P(G)$ is

$$(x+2)^{a+b-2} \det(xI - B),$$

where

$$B = \begin{pmatrix} 2a-2 & b \\ a & 2b-2 \end{pmatrix}.$$

Note that $\mathrm{tr}(B) = 2a + 2b - 4 > 0$ and $\det(B) = 3ab - 4a - 4b + 4$. By defining

$$p(x, y) = 3(x+3)(y+3) - 4(x+3) - 4(y+3) + 3,$$

and using Lemmas 2, we find that $\det(B) > 0$. So the eigenvalues of B are positive. So

$$PE(G) = 2(a+b-2) + \mathrm{tr}(B) = 4a + 4b - 8 = 4n - 8.$$

(ii) Let $v_1, \ldots, v_a$ be the vertices of the cycle of length a, $v_{a+1}, \ldots, v_{a+b}$ be the vertices of the cycle of length b, and $v_{a+b+1}, \ldots, v_{a+b+c}$ be the other vertices of G. The path matrix of G with in this ordering is as follows:

$$P(G) = \begin{pmatrix} 2(J_a - I) & J & J \\ J & 2(J_b - I) & J \\ J & J & J_c - I \end{pmatrix},$$

and by Theorem 1, the characteristic polynomial of $P(G)$ is

$$(x+2)^{a+b-2}(x+1)^{c-1} \det(xI - B),$$

where

$$B = \begin{pmatrix} 2a-2 & b & c \\ a & 2b-2 & c \\ a & b & c-1 \end{pmatrix}.$$

Let $f(x) = \det(xI - B) = x^3 + c_1x^2 + c_2x + c_0 = (x - \lambda_1)(x - \lambda_2)(x - \lambda_3)$, and $\lambda_1 \geq \lambda_2 \geq \lambda_3$. Note that $\lambda_1 > 0$. We have:

$$\lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3 = 3ab + ac + bc - 6a - 6b - 4c + 8.$$

Now by defining

$$p(x, y, z) = 3(x+3)(y+3) + (x+3)(z+1) + (y+3)(z+1) - 6(x+3) - 6(y+3) - 4(z+1) + 7$$

and using Lemma 2, we find that $\lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3 > 0$. If $\lambda_2 \leq 0$, then $\lambda_3 \leq 0$ and $\lambda_1 + \lambda_2 = \mathrm{tr}(B) - \lambda_3 > 0$, which implies that

$$\lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3 = \lambda_1\lambda_2 + (\lambda_1 + \lambda_2)\lambda_3 \leq 0,$$

a contradiction. So, $\lambda_2 > 0$ and f has at most one negative root. On the other hand, the constant term of $f(x-1)$, i.e., minus of the product of its roots, is

$$-(\lambda_1 + 1)(\lambda_2 + 1)(\lambda_3 + 1) = -c(b-1)(a-1) < 0,$$

so $\lambda_3 > -1$. Now, two cases can be considered. If $\lambda_3 \geq 0$, then

$$PE(G) = 2(a+b-2) + (c-1) + \mathrm{tr}(B) = 4a + 4b + 2c - 10 = 4n - 2c - 10,$$

and if $-1 < \lambda_3 \leq 0$, then

$$PE(G) = 2(a+b-2) + (c-1) + \mathrm{tr}(B) - 2\lambda_3 = 4n - 2c - 10 - 2\lambda_3,$$

which implies that $4n - 2c - 10 \leq PE(G) < 4n - 2c - 8$. ■

Corollary 4. *Let G be a bicyclic graph of Type $\mathcal{B}^{(1)}(a,b)$ of order $n = a+b+c$ such that $a, b \geq 4$ and $c \geq 1$, or $a, b \geq 3$ and $c \geq 7$. Then $PE(G) = 4n - 2c - 10$.*

Proof. By the notation used in the proof of Theorem 3,

$$\lambda_1\lambda_2\lambda_3 = -c_0 = abc - 3ab - 2ac - 2bc + 4a + 4b + 4c - 4.$$

By defining

$$\begin{aligned} p(x,y,z) =& (x+4)(y+4)(z+1) - 3(x+4)(y+4) - 2(x+4)(z+1) - 2(y+4)(z+1) + \\ & 4(x+4) + 4(y+4) + 4(z+1) - 4 \end{aligned}$$

and using Lemma 2, we find that for $a, b \geq 4$ and $c \geq 1$, $\lambda_1\lambda_2\lambda_3 \geq 0$. Similarly, for $a, b \geq 3$ and $c \geq 7$, we have $\lambda_1\lambda_2\lambda_3 \geq 0$, and this gives the result. ■

2.2 Bicyclic Graphs of Type $\mathcal{B}^{(2)}$

In this subsection, some bounds on path energy of the second type of bicyclic graphs are obtained.

Theorem 5. *Let $a, b \geq 3$ and G be a bicyclic graph of Type $B^{(2)}(a,b)$ of order $n = a+b+c-1$.*

(i) If $c = 0$, then $|PE(G) - (4n-7)| < 1$.

(ii) If $c > 0$, then $|PE(G) - (4n-2c-6)| < 4$.

Proof. (i) The path matrix of G can be written as follows:

$$P(G) = \begin{pmatrix} 2(J_{a-1} - I) & J & 2J \\ J & 2(J_{b-1} - I) & 2J \\ 2J & 2J & 0_{1\times 1} \end{pmatrix}.$$

Using Theorem 1, the characteristic polynomial of $P(G)$ is

$$(x+2)^{a+b-4} \det(xI - B),$$

where

$$B = \begin{pmatrix} 2a-4 & b-1 & 2 \\ a-1 & 2b-4 & 2 \\ 2a-2 & 2b-2 & 0 \end{pmatrix}.$$

Suppose that $f(x) = \det(xI - B) = (x-\lambda_1)(x-\lambda_2)(x-\lambda_3)$, and $\lambda_1 \geq \lambda_2 \geq \lambda_3$. Note that $\lambda_1 > 0$. On the other hand, $f(-3-x) = -(x^3 + c_1x^2 + c_2x + c_3)$ such that

$$c_1 = 2a + 2b + 1,\ c_2 = 3ab + a + b + 2,\ c_3 = ab + a + b.$$

Thus, for all $x \geq 0$, $f(-3-x) < 0$, which implies that all roots of f are greater than -3. Also, $f(-3) = -ab - a - b < 0$ and $f(-2) = 2ab - 2a - 2b + 2 = 2(a-1)(b-1) > 0$, so by the intermediate value theorem, $\lambda_3 \in (-3, -2)$. The constant term of $f(x)$ is

$$-\lambda_1\lambda_2\lambda_3 = 8ab - 16a - 16b + 24 = 8\left((a-2)(b-2) - 1\right) \geq 0.$$

Therefore $\lambda_2 \geq 0$. Now,

$$PE(G) = 2(a+b-4) + \mathrm{tr}(B) - 2\lambda_3 = 4n - 12 - 2\lambda_3,$$

which implies that, $4n - 8 < PE(G) < 4n - 6$.

(ii) The path matrix of G can be written as follows:

$$P(G) = \begin{pmatrix} 2(J_{a-1} - I) & J & 2J & J \\ J & 2(J_{b-1} - I) & 2J & J \\ 2J & 2J & 0_{1\times 1} & J \\ J & J & J & J_c - I \end{pmatrix}.$$

By Theorem 1, the characteristic polynomial of $P(G)$ is

$$(x+2)^{a+b-4}(x+1)^{c-1} \det(xI - B),$$

where

$$B = \begin{pmatrix} 2a-4 & b-1 & 2 & c \\ a-1 & 2b-4 & 2 & c \\ 2a-2 & 2b-2 & 0 & c \\ a-1 & b-1 & 1 & c-1 \end{pmatrix}.$$

Assume that $f(x) = \det(xI - B) = (x-\lambda_1)(x-\lambda_2)(x-\lambda_3)(x-\lambda_4)$, and $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$. Note that $\lambda_1 > 0$. Let $f(-3-x) = x^4 + c_1x^3 + c_2x^2 + c_3x + c_4$, and

$$c_1 = 2a + 2b + c + 3,$$

$$c_2 = 3ab + ac + bc + 5a + 5b + 2c + 4,$$

$$c_3 = abc + 7ab + ac + bc + 3a + 3b + 2c + 4,$$

$$c_4 = 2ab + ac + bc + 2a + 2b.$$

So, for $x \geq 0$, $f(-3-x) > 0$ which implies that all roots of f are greater than -3. Also, $f(-3) = 2ab + ac + bc + 2a + 2b > 0$ and by Lemma 2, $f(-2) = -abc - 2ab + ac + bc + 2a + 2b - c - 2 < 0$. Now, the intermediate value theorem implies that $\lambda_4 \in (-3, -2)$. Note that the path matrix of Part (i) is a principal sub-matrix of the path matrix of Part (ii). So, if $\lambda_2 < 0$, then by the interlacing theorem [2, p. 17], the path matrix of Part (i) has exactly one non-negative eigenvalue, a contradiction. Thus $\lambda_2 \geq 0$ and

$$\begin{aligned} PE(G) &= 2(a+b-4) + c - 1 + \mathrm{tr}(B) + 2\sum_{\lambda_i<0} |\lambda_i| \\ &= 4n - 2c - 14 + 2\sum_{\lambda_i<0} |\lambda_i| \in (4n-2c-10, 4n-2c-2). \end{aligned}$$

■

In the next theorem, we prove tighter bounds for the path energy of bicyclic graphs of type $\mathcal{B}^{(2)}(3,3)$. These bounds will be used in the next subsection to prove that this type of graph has minimum path energy among bicyclic graphs of the same order.

Theorem 6. *Let G be a graph of order $n \geq 10$ and of Type $\mathcal{B}^{(2)}(3,3)$. Then*

$$2n - 3 + \sqrt{17} - \frac{1}{n} < PE(G) < 2n - 3 + \sqrt{17},$$

in particular, $|PE(G) - (2n + 1.075)| < 0.055$.

Proof. By the notation used in Part (ii) of Theorem 5, the following holds:

$$PE(G) = 2n - 4 + 2\sum_{\lambda_i<0} |\lambda_i|,$$

where $\lambda_1 \geq \lambda_2 \geq \lambda_3$ are the roots of $g(x) = \frac{f(x)}{x}$ (note that 0 is an eigenvalue of B). Since $c = n - 5$, one can see that

$$g(x) = x^3 - (n-2)x^2 - (n+15)x + 4n - 36.$$

Also one can see that,

$$\begin{aligned} g(\frac{-1-\sqrt{17}}{2}) &= 6\sqrt{17} - 26 < 0 \\ g(\frac{-1-\sqrt{17}}{2} + \frac{1}{2n}) &= 7\sqrt{17} - \frac{\sqrt{17}}{4n} - \frac{9}{4n} - \frac{3\sqrt{17}}{8n^2} + \frac{1}{8n^2} + \frac{1}{8n^3} - 26 > 0 \\ g(0) &= 4n - 36 > 0, \\ g(c) &= -4c^2 - 16c - 16 < 0, \\ \lim_{x\to\infty} g(x) &= +\infty, \end{aligned}$$

so g has exactly one negative root contained in $(\frac{-1-\sqrt{17}}{2}, \frac{-1-\sqrt{17}}{2} + \frac{1}{2n})$. Therefore,

$$2n - 3 + \sqrt{17} - \frac{1}{n} < PE(G) < 2n - 3 + \sqrt{17}$$

In particular, since $n \geq 10$, $2n + 1.02 < PE(G) < 2n + 1.13$. ■

2.3 Bicyclic Graphs of Type $\mathcal{B}^{(3)}$

Now, we investigate the last type of bicyclic graphs, $\mathcal{B}^{(3)}$.

Theorem 7. *Let $a, b \geq c + 3$ and G be a bicyclic graph of Type $B^{(3)}(a, b, c)$ of order $n = a + b - c + t - 2$.*

(i) If $t = 0$, then $PE(G) = 2n - 3 + \sqrt{4n^2 - 4n + 17}$,

(ii) If $t > 0$, then $|PE(G) - (4n - 2t - 4)| < 2$.

Proof. (i) Let $c = 0$. The path matrix of G is as follows:

$$P(G) = \begin{pmatrix} 2(J_{a-2} - I) & 2J & 2J \\ 2J & 2(J_{b-2} - I) & 2J \\ 2J & 2J & 3(J_2 - I) \end{pmatrix}.$$

So by Theorem 1, the characteristic polynomial of $P(G)$ can be written as:

$$(x+3)(x+2)^{a+b-6} \det(xI - B),$$

where

$$B = \begin{pmatrix} 2a-6 & 2b-4 & 4 \\ 2a-4 & 2b-6 & 4 \\ 2a-4 & 2b-4 & 3 \end{pmatrix}.$$

The characteristic polynomial of B is as follows:

$$(x+2)(x^2-(2a+2b-7)x-2a-2b+2).$$

If x_1 and x_2 are the roots of $x^2-(2a+2b-7)x-2a-2b+2=0$, then $x_1x_2<0$ and so

$$PE(G)=3+2(a+b-6)+2+|x_1-x_2|.$$

On the other hand,

$$|x_1-x_2|=\sqrt{(x_1+x_2)^2-4x_1x_2}=\sqrt{(2a+2b-7)^2+8(a+b-1)},$$

and $a+b=n+2$, which gives the result.

Now, let $c>0$. The path matrix of G is as follows:

$$P(G)=\begin{pmatrix} 2(J_{a-c-2}-I) & 2J & 2J & 2J \\ 2J & 2(J_{b-c-2}-I) & 2J & 2J \\ 2J & 2J & 3(J_{2\times 2}-I) & 2J \\ 2J & 2J & 2J & 2(J_c-I) \end{pmatrix}.$$

So, using Theorem 1, the characteristic polynomial of $P(G)$ is

$$(x+3)(x+2)^{a+b-c-7}\det(xI-B),$$

where

$$B=\begin{pmatrix} 2a-2c-6 & 2b-2c-4 & 4 & 2c \\ 2a-2c-4 & 2b-2c-6 & 4 & 2c \\ 2a-2c-4 & 2b-2c-4 & 3 & 2c \\ 2a-2c-4 & 2b-2c-4 & 4 & 2c-2 \end{pmatrix}.$$

Consider the characteristic polynomial of B, i.e.,

$$(x+2)^2(x^2-(2a+2b-2c-7)x-2a-2b+2c+2).$$

If x_1,x_2 are the roots of $x^2-(2a+2b-2c-7)x-2a-2b+2c+2=0$, then $x_1x_2<0$. So we find that,

$$PE(G)=3+2(a+b-c-7)+4+|x_1-x_2|.$$

On the other hand,

$$|x_1-x_2|=\sqrt{(x_1+x_2)^2-4x_1x_2}=\sqrt{(2a+2b-2c-7)^2+8(a+b-c-1)},$$

and $a+b-c=n+2$, which implies the result.

(ii) Let $c=0$. The path matrix of G is as follows:

$$P(G)=\begin{pmatrix} 2(J_{a-2}-I) & 2J & 2J & J \\ 2J & 2(J_{b-2}-I) & 2J & J \\ 2J & 2J & 3(J_2-I) & J \\ J & J & J & J_t-I \end{pmatrix}.$$

So, by Theorem 1 we obtain the characteristic polynomial of $P(G)$ as:

$$(x+3)(x+1)^{t-1}(x+2)^{a+b-6}\det(xI-B),$$

where

$$B=\begin{pmatrix} 2a-6 & 2b-4 & 4 & t \\ 2a-4 & 2b-6 & 4 & t \\ 2a-4 & 2b-4 & 3 & t \\ a-2 & b-2 & 2 & t-1 \end{pmatrix}.$$

Let $f(x)=\det(xI-B)$. Note that -2 is a root of $f(x)$. Suppose that $f(x)=(x+2)g(x)$. One can see that $g(-2-x)=-(x^3+c_1x^2+c_2x+c_3)$, where

$$c_1=2a+2b+t-2,$$

$$c_2=at+bt+4a+4b-t-11,$$

$$c_3=at+bt+2a+2b-4t-8.$$

Note that $c_1,c_2,c_3>0$, so for $x\geq 0$, $g(-2-x)<0$, which implies that the roots of $g(x)$ are contained in $(-2,\infty)$. Let $\lambda_1\geq\lambda_2\geq\lambda_3$ be the roots of $g(x)$. Note that $\lambda_1>0$ and,

$$\begin{aligned} PE(G) &= 3+(t-1)+2(a+b-6)+\mathrm{tr}(B)+4+2\sum_{\lambda_i<0}|\lambda_i| \\ &= 4n-2t-8+2\sum_{\lambda_i<0}|\lambda_i|. \end{aligned}$$

Also we have,

$$g(-2)=-at-bt-2a-2b+4t+8=-t(a+b-4)-2(a+b-4)<0,$$

$$g(-1)=2t>0,$$

so g has an odd number of roots (including multiplicities) in $(-2,-1)$. Since $\lambda_1>0$, there is exactly one root of g in $(-2,-1)$. Therefore, $-2<\lambda_3<-1<\lambda_2$, which yields that $1<\sum_{\lambda_i<0}|\lambda_i|<3$, and so

$$4n-2t-6<PE(G)<4n-2t-2.$$

Now, let $c>0$. The path matrix of G is as follows:

$$P(G)=\begin{pmatrix} 2(J_{a-c-2}-I) & 2J & 2J & 2J & J \\ 2J & 2(J_{b-c-2}-I) & 2J & 2J & J \\ 2J & 2J & 3(J_2-I) & 2J & J \\ 2J & 2J & 2J & 2(J_c-I) & J \\ J & J & J & J & J_t-I \end{pmatrix}.$$

Using Theorem 1, the characteristic polynomial of $P(G)$ is as follows:

$$(x+3)(x+2)^{a+b-c-7}(x+1)^{t-1}\det(xI-B),$$

where

$$B=\begin{pmatrix} 2a-2c-6 & 2b-2c-4 & 4 & 2c & t \\ 2a-2c-4 & 2b-2c-6 & 4 & 2c & t \\ 2a-2c-4 & 2b-2c-4 & 3 & 2c & t \\ 2a-2c-4 & 2b-2c-4 & 4 & 2c-2 & t \\ a-c-2 & b-c-2 & 2 & c & t-1 \end{pmatrix}.$$

The first three rows of $B+2I$ are the same. Hence, $\operatorname{rank}(B+2I)\leq 3$ and so $\operatorname{null}(B+2I)\geq 2$, which implies that -2 is an eigenvalue of B with multiplicity at least 2. Let $f(x)=\det(xI-B)=(x+2)^2g(x)$. Suppose that $g(-2-x)=-(x^3+c_1x^2+c_2x+c_3)$, where

$$\begin{aligned} c_1 &= 2a+2b-2c+t-2, \\ c_2 &= at+bt-ct+4a+4b-4c-t-11, \\ c_3 &= at+bt-ct+2a+2b-2c-4t-8. \end{aligned}$$

Since $a+b-c\geq 6$, $c_1,c_2,c_3>0$. Thus, for $x\geq 0$, $g(-2-x)<0$, therefore the roots of $g(x)$ are contained in $(-2,\infty)$. Let $\lambda_1\geq\lambda_2\geq\lambda_3$ be the roots of $g(x)$. We have

$$\begin{aligned} PE(G) &= 3+(t-1)+2(a+b-c-7)+\operatorname{tr}(B)+8+2\sum_{\lambda_i<0}|\lambda_i| \\ &= 4n-2t-8+2\sum_{\lambda_i<0}|\lambda_i|. \end{aligned}$$

Since

$$\begin{aligned} g(-2) &= -(t+2)(a+b-c-4)=-(t+2)(n-t-2)<0, \\ g(-1) &= 2t>0, \end{aligned}$$

so g has an odd number of roots (including multiplicities) in $(-2,-1)$. Also $\lambda_1>0$, hence g has exactly one root in $(-2,-1)$. Therefore $-2<\lambda_3<-1<\lambda_2$, which implies that $1<\sum_{\lambda_i<0}|\lambda_i|<3$, and

$$4n-2t-6<PE(G)<4n-2t-2.$$

This completes the proof. ■

3 Bicyclic Graphs with Maximum and Minimum Path Energy

In this section, we obtain the types of bicyclic graphs with a fixed order which attain the maximum and minimum values of path energy. Using these, one can see that the Conjectures 1 and 2 are valid. First consider bicyclic graphs with the maximum path energy.

Theorem 8. *Among all bicyclic graphs of order $n \geq 4$, a graph of type $\mathcal{B}^{(3)}(a, b, c)$, with $n = a + b - c - 2$ has maximum path energy.*

Proof. Let G be a bicyclic graph of Type $\mathcal{B}^{(3)}(a, b, c)$ with $n = a+b-c-2$. By Theorem 7,

$$PE(G) = 2n - 3 + \sqrt{4n^2 - 4n + 17} > 2n - 3 + \sqrt{4n^2 - 4n + 1} = 4n - 4.$$

On the other hand, by Theorems 3, 5, and 7, the path energy of all other types of bicyclic graphs of order n is less than $4n - 4$. ■

Now, in the class of bicyclic graphs with the same order, we identify the graph with minimum path energy.

Theorem 9. *Among all bicyclic graphs of order $n \geq 5$, a graph of Type $\mathcal{B}^{(2)}(3, 3)$ has minimum path energy.*

Proof. A computer search shows that the result holds for $5 \leq n \leq 9$. So, suppose that $n \geq 10$ and H be a bicyclic graph of order n and of Type $\mathcal{B}^{(2)}(3, 3)$. Let G be a bicyclic graph of order n and of Type $\mathcal{B}^{(1)}(a, b)$. By Theorems 3 and 6, if $c = n - a - b = 0$, then

$$PE(G) = 4n - 8 > 2n + 1.13 > PE(H).$$

Also if $c > 0$, then $c \leq n - 6$ and

$$PE(G) \geq 4n - 2c - 10 \geq 4n - 2(n - 6) - 10 > 2n + 1.13 > PE(H).$$

Now, let G be a bicyclic graph of order n and of Type $\mathcal{B}^{(2)}(a, b)$. By Theorems 5 and 6, if $c = n - a - b + 1 = 0$ then

$$PE(G) > 4n - 8 > 2n + 1.13 > PE(H).$$

Also if $c > 0$ and at least one of the a and b is greater than 3, then $n \geq c + 6$ and

$$PE(G) > 4n - 2c - 10 \geq 4n - 2(n-6) - 10 > 2n + 1.13 > PE(H).$$

Finally, let G be a bicyclic graph of order n and of Type $\mathcal{B}^{(3)}(a, b, c)$. By Theorems 6 and 7, if $t = n - a - b + c + 2 = 0$, then

$$PE(G) = 2n - 3 + \sqrt{4n^2 - 4n + 17} \geq 2n + 1.13 > PE(H).$$

If $t > 0$, then $n \geq t + 4$ and by Theorems 6 and 7 we have:

$$PE(G) > 4n - 2t - 6 \geq 4n - 2(n-4) - 6 > 2n + 1.13 > PE(H).$$

The proof is complete. ■

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