Solution to a conjecture on the maximal energy of bipartite bicyclic graphs∗

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Abstract

The energy of a simple graph $G$, denoted by $E(G)$, is defined as the sum of the absolute values of all eigenvalues of its adjacency matrix. Let $C_n$ denote the cycle of order $n$ and $P_n^{6,6}$ the graph obtained from joining two cycles $C_6$ by a path $P_{n-12}$ with its two leaves. Let $B_n$ denote the class of all bipartite bicyclic graphs but not the graph $R_{a,b}$, which is obtained from joining two cycles $C_a$ and $C_b$ ($a, b \geq 10$ and $a \equiv b \equiv 2 \pmod{4}$) by an edge. In [I. Gutman, D. Vidović, Quest for molecular graphs with maximal energy: a computer experiment, J. Chem. Inf. Sci. 41 (2001), 1002–1005], Gutman and Vidović conjectured that the bicyclic graph with maximal energy is $P_n^{6,6}$, for $n = 14$ and $n \geq 16$. In [X. Li, J. Zhang, On bicyclic graphs with maximal energy, Linear Algebra Appl. 427 (2007), 87–98], Li and Zhang showed that the conjecture is true for graphs in the class $B_n$. However, they could not determine which of the two graphs $R_{a,b}$ and $P_n^{6,6}$ has the maximal value of energy. In [B. Furtula, S. Radenković, I. Gutman, Bicyclic molecular graphs with the greatest energy, J. Serb. Chem. Soc. 73(4) (2008), 431–433], numerical computations up to $a + b = 50$ were reported, supporting the conjecture. So, it is still necessary to have a mathematical proof to this conjecture. This paper is to show that the energy of $P_n^{6,6}$ is larger than that of $R_{a,b}$, which proves the conjecture for bipartite bicyclic graphs. For non-bipartite bicyclic graphs, the conjecture is still open.

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1 Introduction

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

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

(1.1)

The roots $\lambda_1, \lambda_2, \ldots, \lambda_n$ of $\phi(G, x) = 0$ are called the eigenvalues of $G$.

If $G$ is a bipartite graph, the characteristic polynomial of $G$ has the form

$$
\phi(G, x) = \left\lfloor \frac{n}{2} \right\rfloor \sum_{k=0}^{\left\lfloor \frac{n}{2} \right\rfloor} a_{2k} x^{n-2k} = \sum_{k=0}^{\left\lfloor \frac{n}{2} \right\rfloor} (-1)^k b_{2k} x^{n-2k},
$$

where $b_{2k} = (-1)^k a_{2k}$ for all $k = 1, \ldots, \left\lfloor \frac{n}{2} \right\rfloor$, especially $b_0 = a_0 = 1$. In particular, if $G$ is a tree, the characteristic polynomial of $G$ can be expressed as

$$
\phi(G, x) = \sum_{k=0}^{\left\lfloor \frac{n}{2} \right\rfloor} (-1)^k m(G, k) x^{n-2k},
$$

where $m(G, k)$ is the number of $k$-matchings of $G$.

In the following, two basic properties of the characteristic polynomial $\phi(G)$ \[1\] will be stated:

**Proposition 1.1** If $G_1, G_2, \ldots, G_r$ are the connected components of a graph $G$, then

$$
\phi(G) = \prod_{i=1}^{r} \phi(G_i).
$$

**Proposition 1.2** Let $uv$ be an edge of $G$. Then

$$
\phi(G, x) = \phi(G - uv, x) - \phi(G - u - v, x) - 2 \sum_{C \in \mathcal{C}(uv)} \phi(G - C, x),
$$

where $\mathcal{C}(uv)$ is the set of cycles containing $uv$. In particular, if $uv$ is a pendent edge with pendent vertex $v$, then $\phi(G, x) = x \phi(G - v, x) - \phi(G - u - v, x)$.

The energy of $G$, denoted by $E(G)$, is defined as $E(G) = \sum_{i=0}^{n} |\lambda_i|$. This definition was proposed by Gutman \[4\]. The following formula is also well-known

$$
E(G) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \log |x^n \phi(G, i/x)| \, dx,
$$
where \( i^2 = -1 \). Moreover, it is known from [1] that the above equality can be expressed as the following explicit formula:

\[
E(G) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \log \left[ \left( \sum_{i=0}^{\lfloor n/2 \rfloor} (-1)^i a_{2i} x^{2i} \right)^2 + \left( \sum_{i=0}^{\lfloor n/2 \rfloor} (-1)^i a_{2i+1} x^{2i+1} \right)^2 \right] dx,
\]

where \( a_1, a_2, \ldots, a_n \) are the coefficients of the characteristic polynomial \( \phi(G, x) \). For more results about graph energy, we refer the readers to a survey of Gutman, Li and Zhang [9].

Since 1980s, the extremal energy \( E(G) \) of a graph \( G \) has been studied extensively, but the common method makes use of the quasi-order. When the graphs are acyclic, bipartite or unicyclic, it is almost always valid. However, for general graphs, the quasi-order method is invalid. Recently, for these quasi-order incomparable problems, we found an efficient way to determine which one attains the extremal value of the energy, see [11–16], especially, in [15] we completely solved a conjecture that \( P_{6}^n \) has the maximal energy among all unicyclic graphs of order \( n \geq 16 \).

In this paper, graphs under our consideration are finite, connected and simple. Let \( P_n \) and \( C_n \) denote the path and cycle with \( n \) vertices, respectively. Let \( P_n^t \) be the unicyclic graph obtained by joining a vertex of \( C_t \) with a leaf of \( P_{n-t} \), and \( P_n^6,6 \) the graph obtained from joining two cycles \( C_6 \) by a path \( P_{n-12} \) with its two leaves. Denote by \( R_{a,b} \) the graph obtained from connecting two cycles \( C_a \) and \( C_b \) (\( a, b \geq 10 \) and \( a \equiv b \equiv 2 \pmod{4} \)) by an edge. Let \( \mathcal{B}_n \) be the class of all bipartite bicyclic graphs but not the graph \( R_{a,b} \). In [8], Gutman and Vidović proposed the following conjecture on bicyclic graphs with maximal energy:

**Conjecture 1.3** For \( n = 14 \) and \( n \geq 16 \), the bicyclic molecular graph of order \( n \) with maximal energy is the molecular graph of the \( \alpha, \beta \) diphenyl-polyene \( C_6H_5(CH)_{n-12}C_6H_5 \), or denoted by \( P_n^{6,6} \).

For bipartite bicyclic graphs, Li and Zhang in [17] got the following result, giving a partial solution to the above conjecture.

**Theorem 1.4** If \( G \in \mathcal{B}_n \), then \( E(G) \leq E(P_n^{6,6}) \) with equality if and only if \( G \cong P_n^{6,6} \).

However, they could not compare the energies of \( P_n^{6,6} \) and \( R_{a,b} \). Furtula et al. in [3] showed that \( E(P_n^{6,6}) > E(R_{a,b}) \) by numerical computations up to \( a + b = 50 \), supporting that the conjecture is true for bipartite bicyclic graphs. It is evident that a mathematical proof is still needed. This paper is to give such a proof. We will use Coulson integral formula and some knowledge of real analysis as well as combinatorial method to show the following result:

**Theorem 1.5** For \( n - t, t \geq 10 \) and \( n - t \equiv t \equiv 2 \pmod{4} \), \( E(R_{n-t,t}) < E(P_n^{6,6}) \).
As Furtula et al. noticed in [3], since for odd \( n \) the graph \( R_{a,b} \) \( (a + b = n) \) is not bipartite, therefore, for odd \( n \), it is known that \( P_n^{6,6} \) is the maximal energy bipartite bicyclic graph from [17]. Therefore, combining Theorems 1.4 and 1.5 we get:

**Theorem 1.6** Let \( G \) be any connected, bipartite bicyclic graph with \( n \) \((n \geq 12)\) vertices. Then \( E(G) \leq E(P_n^{6,6}) \) with equality if and only if \( G \cong P_n^{6,6} \).

So, Conjecture 1.3 is true for all connected bipartite bicyclic graphs of order \( n \) with \( n = 14 \) and \( n \geq 16 \). However, it is still open for non-bipartite bicyclic graphs.

2 Proof of Theorem 1.5

Before giving the proof of Theorem 1.5, we shall state some knowledge on real analysis [20].

**Lemma 2.1** For any real number \( X > -1 \), we have

\[
\frac{X}{1 + X} \leq \log(1 + X) \leq X.
\]

In particular, \( \log(1 + X) < 0 \) if and only if \( X < 0 \).

The following lemma is a well-known conclusion due to Gutman [6] which will be used later.

**Lemma 2.2** If \( G_1 \) and \( G_2 \) are two graphs with the same number of vertices, then

\[
E(G_1) - E(G_2) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \log \frac{\phi(G_1; ix)}{\phi(G_2; ix)} dx.
\]

One can easily obtain the following recursive equations from Propositions 1.1 and 1.2.

**Lemma 2.3** For any positive number \( n \geq 8 \),

\[
\begin{align*}
\phi(P_n, x) &= x\phi(P_{n-1}, x) - \phi(P_{n-2}, x), \\
\phi(C_n, x) &= \phi(P_n, x) - \phi(P_{n-2}, x) - 2, \\
\phi(P_n^6, x) &= x\phi(P_{n-1}^6, x) - \phi(P_{n-2}^6, x);
\end{align*}
\]

for any positive number \( n \geq 6 \) and \( t \geq 3 \),

\[
\phi(R_{n-t,t}, x) = \phi(C_{n-t}, x)\phi(C_t, x) - \phi(P_{n-t-1}, x)\phi(P_{t-1}, x).
\]
Next, we introduce some convenient notations as follows, which will be used in the sequel.

\[ Y_1(x) = \frac{x + \sqrt{x^2 - 4}}{2}, \quad Y_2(x) = \frac{x - \sqrt{x^2 - 4}}{2}. \]

It is easy to verify that \( Y_1(x) + Y_2(x) = x, \) \( Y_1(x)Y_2(x) = 1, \) \( Y_1(ix) = \frac{x + \sqrt{x^2 + 4}}{2}i \) and \( Y_2(ix) = \frac{x - \sqrt{x^2 + 4}}{2}i. \) Furthermore, we define

\[ Z_1(x) = -iY_1(ix) = \frac{x + \sqrt{x^2 + 4}}{2}, \quad Z_2(x) = -iY_2(ix) = \frac{x - \sqrt{x^2 + 4}}{2}. \]

Note that \( Z_1(x) + Z_2(x) = x, \) \( Z_1(x)Z_2(x) = -1. \) Moreover, \( Z_1(x) > 1 \) and \( -1 < Z_2(x) < 0, \) if \( x > 0; \) \( 0 < Z_1(x) < 1 \) and \( Z_2(x) < -1, \) otherwise. In the rest of this paper, we abbreviate \( Z_j(x) \) to \( Z_j \) for \( j = 1, 2. \) Some more notations will be used frequently in the sequel.

\[
A_1(x) = \frac{Y_1(x)\phi(P_{13}^{6,6}, x) - \phi(P_{13}^{6,6}, x)}{(Y_1(x))^{14} - (Y_1(x))^{12}}, \quad A_2(x) = \frac{Y_2(x)\phi(P_{13}^{6,6}, x) - \phi(P_{13}^{6,6}, x)}{(Y_2(x))^{14} - (Y_2(x))^{12}}, \\
B_1(x) = \frac{Y_1(x)(x^2 - 1) - x}{(Y_1(x))^3 - Y_1(x)}, \quad B_2(x) = \frac{Y_2(x)(x^2 - 1) - x}{(Y_2(x))^3 - Y_2(x)}.
\]

By some simple calculations, we have that \( \phi(P_{13}^{6,6}, x) = x^{13} - 14x^{11} + 74x^9 - 188x^7 + 245x^5 - 158x^3 + 40x \) and \( \phi(P_{12}^{6,6}, x) = x^{12} - 13x^{10} + 62x^8 - 138x^6 + 153x^4 - 81x^2 + 16, \) and then

\[ A_1(ix) = \frac{Z_1g_{13} + g_{12}Z_2}{Z_1^2 + 1}, \quad A_2(ix) = \frac{Z_2g_{13} + g_{12}Z_1}{Z_2^2 + 1}, \]

where \( g_{13} = x^{13} + 14x^{11} + 74x^9 + 188x^7 + 245x^5 + 158x^3 + 40x \) and \( g_{12} = x^{12} + 13x^{10} + 62x^8 + 138x^6 + 153x^4 + 81x^2 + 16. \) Notice that \( A_j(ix) \) has a good property, i.e., its sign is always positive for all real number \( x, \) for \( j = 1, 2. \)

**Observation 2.4** For all real number \( x, \) \( A_j(ix) > 0, \) \( j = 1, 2. \)

**Proof.** Since, by some directed calculations, we have

\[ A_1(ix)A_2(ix) = \frac{(x^6 + 8x^4 + 19x^2 + 16)^2(x^2 + 1)^4}{x^2 + 4} > 0 \text{ for all } x. \]

Besides, from the expression of \( A_1(ix), \) we obviously obtain that \( A_1(ix) > 0 \) for all real \( x. \) Thus, we conclude that \( A_2(ix) > 0. \) For convenience, we abbreviate \( A_j(ix) \) and \( C_j(ix) \) to \( A_j \) and \( C_j \) for \( j = 1, 2, \) respectively.

The following lemma will be used in the showing of the later results, due to Huo et al. [13–15].

**Lemma 2.5** For \( n \geq 4 \) and \( x \neq \pm 2, \) the characteristic polynomials of \( P_n \) and \( C_n \) possess the following forms:

\[
\phi(P_n, x) = B_1(x)(Y_1(x))^n + B_2(x)(Y_2(x))^n
\]
and

\[ \phi(C_n, x) = (Y_1(x))^n + (Y_2(x))^n - 2. \]

**Lemma 2.6** For \( n \geq 12 \), the characteristic polynomial of \( P_{n}^{6,6} \) has the following form:

\[ \phi(P_{n}^{6,6}, x) = A_1(x)(Y_1(x))^n + A_2(x)(Y_2(x))^n \]

where \( x \neq \pm 2 \).

**Proof.** Note that, \( \phi(P_{n}^{6,6}) \) satisfies the recursive formula \( f(n, x) = xf(n - 1, x) - f(n - 2, x) \) in terms of Lemma 2.3. Therefore, the form of the general solution of the linear homogeneous recursive relation is \( f(n, x) = D_1(x)(Y_1(x))^n + D_2(x)(Y_2(x))^n \). By some simple calculations, together with the initial values \( \phi(P_{12}^{6,6}) \) and \( \phi(P_{13}^{6,6}) \), we can get that \( D_i(x) = A_i(x), i = 1, 2 \).

From Lemmas 2.3 and 2.5 and Proposition 1.1 by means of elementary calculations it is easy to deduce the following result. The details of its proof is omitted.

**Lemma 2.7** For \( n \geq 6 \) and \( t \geq 3 \), the characteristic polynomial of \( R_{n-t,t} \) has the following form:

\[ \phi(R_{n-t,t}, x) = C_1(x)(Y_1(x))^n + C_2(x)(Y_2(x))^n - 2((Y_1(x))^t + (Y_2(x))^t) + 4 \]

where \( x \neq \pm 2 \), \( C_1(x) = 1 + (Y_2(x))^{2t} - 2(Y_2(x))^t - (B_1(x))^2(Y_2(x))^2 - B_1(x)B_2(x)(Y_2(x))^{2t} \) and \( C_2(x) = 1 + (Y_1(x))^{2t} - 2(Y_1(x))^t - (B_2(x))^2(Y_1(x))^2 - B_1(x)B_2(x)(Y_1(x))^{2t} \).

In terms of the above lemma, we can get the following forms for \( C_j(ix) (j = 1, 2) \) by some simplifications,

\[ C_1(ix) = 1 + \frac{x^2 + 3}{x^2 + 4} Z_2^{2t} + 2 Z_1^t + \frac{Z_1^2}{(Z_2^2 + 1)^2} \]

\[ C_2(ix) = 1 + \frac{x^2 + 3}{x^2 + 4} Z_1^{2t} + 2 Z_2^t + \frac{Z_2^2}{(Z_1^2 + 1)^2}. \]

**Proof of Theorem 1.5**

From the above analysis, we only need to show that \( E(R_{n-t,t}) < E(P_{n}^{6,6}) \), for every positive number \( t = 4k_1 + 2 \) \( (t \geq 10) \), \( n - t \geq 10 \) and \( n = 4k_2 \) \( (n \geq 2t) \). Without loss of generality, we assume \( n - t \geq t \), that is, \( n \geq 2t \). From Lemma 2.2 we have that

\[ E(R_{n-t,t}) - E(P_{n}^{6,6}) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\phi(R_{n-t,t}; ix)}{\phi(P_{n}^{6,6}; ix)} \, dx. \]
First of all, we shall will that the integrand \( \log \frac{\phi(R_{n-t,t}; ix)}{\phi(P_{n-4}; ix)} \) is monotonically decreasing in \( n \) for \( n = 4k \), that is,

\[
\log \frac{\phi(R_{n+4-t,t}; ix)}{\phi(P_{n+4}; ix)} - \log \frac{\phi(R_{n-t,t}; ix)}{\phi(P_{n}; ix)} = \log \frac{\phi(R_{n+4-t,t}; ix)\phi(P_{n}; ix)}{\phi(R_{n-t,t}; ix)} = \log \left( 1 + \frac{K(n, t, x)}{H(n, t, x)} \right),
\]

where \( K(n, t, x) = \phi(R_{n+4-t,t}; ix)\phi(P_{n}; ix) - \phi(P_{n+4}; ix)\phi(R_{n-t,t}; ix) \) and \( H(n, t, x) = \phi(P_{n+4}; ix)\phi(R_{n-t,t}; ix) > 0 \). From Lemma 2.1, we only need to verify that \( K(n, t, x) < 0 \). By means of some directed calculations, we arrive at

\[
K(n, t, x) = (Z_{1}^{2} - Z_{2}^{2})(A_{2}C_{1} - A_{1}C_{2}) + (2Z_{1} + 2Z_{2}^t + 4)(A_{1}Z_{1}^n(1 - Z_{1}^{4}) + A_{2}Z_{2}^n(1 - Z_{2}^{4})).
\]

Noticing that \( Z_{1} > 1 \) and \( 0 > Z_{2} > -1 \) for \( x > 0 \), we have \( Z_{1}^{n} \geq Z_{1}^{2t} > 0 \) and \( 0 < Z_{2}^t \leq Z_{2}^{2t} \). Meanwhile, from \( 0 < Z_{1} < 1 \) and \( Z_{2} < -1 \) for \( x < 0 \), we have \( 0 < Z_{1}^{n} \leq Z_{1}^{2t} \) and \( Z_{2}^t \geq Z_{2}^{2t} > 0 \). Therefore,

\[
A_{1}Z_{1}^n(1 - Z_{1}^{4}) + A_{2}Z_{2}^n(1 - Z_{2}^{4}) \leq A_{1}Z_{1}^n(1 - Z_{1}^{2t}) + A_{2}Z_{2}^n(1 - Z_{2}^{2t}).
\]

Namely, \( K(n, t, x) \leq K(2t, t, x) = (Z_{1}^{4} - Z_{2}^{4})(A_{2}C_{1} - A_{1}C_{2}) + (2Z_{1} + 2Z_{2}^t + 4)(A_{1}Z_{1}^2(1 - Z_{1}^{4}) + A_{2}Z_{2}^2(1 - Z_{2}^{4})) \). Now let \( f(t, x) = K(2t, t, x) \). By some simplifications, it is easy to get

\[
f(t, x) = \alpha_{0}Z_{1}^{3t} + \alpha_{1}Z_{1}^{-3t} + \beta_{0}Z_{1}^{2t} + \beta_{1}Z_{1}^{-2t} + \gamma_{0}Z_{1}^{t} + \gamma_{1}Z_{1}^{-t} + a_{0},
\]

where

\[
\begin{align*}
\alpha_{0} &= 2A_{1}(1 - Z_{1}^{4}), \\
\alpha_{1} &= 2A_{2}(1 - Z_{2}^{4}), \\
\beta_{0} &= A_{1}\left(4(1 - Z_{1}^{4}) - (Z_{1}^{4} - Z_{2}^{4})\frac{x^2 + 3}{x^2 + 4}\right), \\
\beta_{1} &= A_{2}\left(4(1 - Z_{2}^{4}) + (Z_{1}^{4} - Z_{2}^{4})\frac{x^2 + 3}{x^2 + 4}\right), \\
\gamma_{0} &= 2A_{1}((1 - Z_{1}^{4}) - (Z_{1}^{4} - Z_{2}^{4})), \\
\gamma_{1} &= 2A_{2}((1 - Z_{2}^{4}) + (Z_{1}^{4} - Z_{2}^{4})),
\end{align*}
\]

and

\[
a_{0} = (Z_{1}^{4} - Z_{2}^{4})\left(A_{2}\left(1 + \frac{Z_{2}^{3}}{(Z_{2}^{2} + 1)^2}\right) - A_{1}\left(1 + \frac{Z_{2}^{3}}{(Z_{2}^{2} + 1)^2}\right)\right).
\]

**Claim 1.** \( f(t, x) \) is monotonically decreasing in \( t \).

Note the facts that \( (1 - Z_{1}^{4}) < 0 \) for \( x > 0 \), \( (1 - Z_{1}^{4}) > 0 \) for \( x < 0 \); \( (1 - Z_{2}^{4}) > 0 \) for \( x > 0 \), \( (1 - Z_{2}^{4}) < 0 \) for \( x < 0 \); \( (Z_{1}^{4} - Z_{2}^{4}) > 0 \) for \( x > 0 \), \( (Z_{1}^{4} - Z_{2}^{4}) < 0 \) for \( x < 0 \). It is not difficult to check that \( \alpha_{0} < 0, \beta_{0} < 0 \) and \( \gamma_{0} < 0 \) for \( x > 0 \), \( \alpha_{0} > 0, \beta_{0} > 0 \) and \( \gamma_{0} > 0 \), otherwise; thus \( \alpha_{1} > 0, \beta_{1} > 0 \) and \( \gamma_{1} > 0 \) for \( x > 0 \), \( \alpha_{1} < 0, \beta_{1} < 0 \) and \( \gamma_{1} < 0 \), otherwise. Therefore, no matter which of \( x > 0 \) or \( x < 0 \) happens, we can always deduce that

\[
\frac{\partial f(t, x)}{\partial t} = (3\alpha_{0}Z_{1}^{3t} - 3\alpha_{1}Z_{1}^{-3t} + 2\beta_{0}Z_{1}^{2t} - 2\beta_{0}Z_{1}^{-2t} + \gamma_{0}Z_{1}^{t} - \gamma_{1}Z_{1}^{-t})\log Z_{1} < 0.
\]
The proof of Claim 1 is thus complete.

From Claim 1, it follows that for \( t \geq 10, \)

\[
K(n, t, x) \leq f(10, x) = -4x^2(x^2 + 1)^2(x^{18} + 23x^{16} + 224x^{14} + 1203x^{12} + 3887x^{10} + 7731x^8 + 9285x^6 + 6301x^4 + 2077x^2 + 224) - (x^{10} + 13x^8 + 62x^6 + 131x^4 + 109x^2 + 16) 
\times x^2(x^4 + 5x^2 + 6)(x^4 + 3x^2 + 1)(x^2 + 1)^2 < 0.
\]

Therefore, we have verified that the integrand \( \log \frac{\phi(R_{n-t,t};ix)}{\phi(P_{n,t};ix)} \) is monotonically decreasing in \( n \) for \( n = 4k \). That is, \( E(R_{n-t,t}) - E(P_{n,6}) \leq E(R_{10,10}) - E(P_{12,6}) < 0 \) for every positive number \( t = 4k_1 + 2 (n \geq 10), n - t \geq 10 \) and \( n = 4k_2 (n \geq 2t) \). Therefore, the entire proof of Theorem 1.5 is now complete.

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