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 $\mathscr{B}_n$ 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 $\mathscr{B}_n$. 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

$$\phi(G,x) = det(xI - A(G)) = \sum_{i=0}^{n} a_i x^{n-i}. \qquad (1.1)$$

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

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

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

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

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

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \log |x^n \phi(G, i/x)| \mathrm{d}x,$$

where $i^2 = -1$. Moreover, it is known from [1] that the above equality can be expressed as the following explicit formula:

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

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_n^6 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^ℓ be the unicyclic graph obtained by joining a vertex of C_ℓ with a leaf of $P_{n-\ell}$, 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 $\mathscr{B}_n$ 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 α, β 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 $G \in \mathscr{B}_n$, 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*

$$E(G_1) - E(G_2) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \log \frac{\phi(G_1; ix)}{\phi(G_2; ix)} \mathrm{d}x.$$

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

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

$$\begin{aligned}
\phi(P_n, x) &= x\phi(P_{n-1}, x) - \phi(P_{n-2}, x),\\
\phi(C_n, x) &= \phi(P_n, x) - \phi(P_{n-2}, x) - 2,\\
\phi(P_n^6, x) &= x\phi(P_{n-1}^6, x) - \phi(P_{n-2}^6, x);
\end{aligned}$$

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.

$$Y_1(x) = \frac{x+\sqrt{x^2-4}}{2}, \qquad Y_2(x) = \frac{x-\sqrt{x^2-4}}{2}.$$

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.

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

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

$$A_1(ix) = \frac{Z_1 g_{13} + g_{12}}{Z_1^2 + 1} Z_2^{12}, \qquad A_2(ix) = \frac{Z_2 g_{13} + g_{12}}{Z_1^2 + 1} Z_1^{12},$$

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,

$$C_1(ix) = 1 + \frac{x^2+3}{x^2+4}Z_2^{2t} + 2Z_2^t + \frac{Z_1^2}{(Z_1^2+1)^2}$$
$$C_2(ix) = 1 + \frac{x^2+3}{x^2+4}Z_1^{2t} + 2Z_1^t + \frac{Z_2^2}{(Z_2^2+1)^2}.$$

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

$$E(R_{n-t,t}) - E(P_n^{6,6}) = \frac{1}{\pi}\int_{-\infty}^{+\infty} \log \frac{\phi(R_{n-t,t}; ix)}{\phi(P_n^{6,6}; ix)} \mathrm{d}x.$$

First of all, we shall will that the integrand $\log \frac{\phi(R_{n-t,t};ix)}{\phi(P_n^{6,6};ix)}$ is monotonically decreasing in n for $n = 4k$, that is,

$$\begin{aligned}
&\log \frac{\phi(R_{n+4-t,t};ix)}{\phi(P_{n+4}^{6,6};ix)} - \log \frac{\phi(R_{n-t,t};ix)}{\phi(P_n^{6,6};ix)} \\
&= \log \frac{\phi(R_{n+4-t,t};ix)\phi(P_n^{6,6};ix)}{\phi(P_{n+4}^{6,6};ix)\phi(R_{n-t,t};ix)} = \log\left(1 + \frac{K(n,t,x)}{H(n,t,x)}\right),
\end{aligned}$$

where $K(n,t,x) = \phi(R_{n+4-t,t};ix)\phi(P_n^{6,6};ix) - \phi(P_{n+4}^{6,6};ix)\phi(R_{n-t,t};ix)$ and $H(n,t,x) = \phi(P_{n+4}^{6,6};ix)\phi(R_{n-t,t};ix) > 0$. From Lemma 2.1, we only need to verify that $K(n,t,x) < 0$. By means of some directed calculations, we arrive at

$$K(n,t,x) = (Z_1^4 - Z_2^4)(A_2C_1 - A_1C_2) + (2Z_1^t + 2Z_2^t + 4)(A_1Z_1^n(1 - Z_1^4) + A_2Z_2^n(1 - Z_2^4)).$$

Noticing that $Z_1 > 1$ and $0 > Z_2 > -1$ for $x > 0$, we have $Z_1^n \geq Z_1^{2t} > 0$ and $0 < Z_2^n \leq Z_2^{2t}$. Meanwhile, from $0 < Z_1 < 1$ and $Z_2 < -1$ for $x < 0$, we have $0 < Z_1^n \leq Z_1^{2t}$ and $Z_2^n \geq Z_2^{2t} > 0$. Therefore,

$$A_1Z_1^n(1 - Z_1^4) + A_2Z_2^n(1 - Z_2^4) \leq A_1Z_1^{2t}(1 - Z_1^4) + A_2Z_2^{2t}(1 - Z_2^4).$$

Namely, $K(n,t,x) \leq K(2t,t,x) = (Z_1^4 - Z_2^4)(A_2C_1 - A_1C_2) + (2Z_1^t + 2Z_2^t + 4)(A_1Z_1^{2t}(1 - Z_1^4) + A_2Z_2^{2t}(1 - Z_2^4))$. 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

$$\begin{aligned}
\alpha_0 &= 2A_1(1 - Z_1^4), & \alpha_1 &= 2A_2(1 - Z_2^4),\\
\beta_0 &= A_1\left(4(1 - Z_1^4) - (Z_1^4 - Z_2^4)\frac{x^2+3}{x^2+4}\right), & \beta_1 &= A_2\left(4(1 - Z_2^4) + (Z_1^4 - Z_2^4)\frac{x^2+3}{x^2+4}\right),\\
\gamma_0 &= 2A_1((1 - Z_1^4) - (Z_1^4 - Z_2^4)), & \gamma_1 &= 2A_2((1 - Z_2^4) + (Z_1^4 - Z_2^4)),
\end{aligned}$$

and

$$a_0 = (Z_1^4 - Z_2^4)\left(A_2\left(1 + \frac{Z_1^2}{(Z_1^2+1)^2}\right) - A_1\left(1 + \frac{Z_2^2}{(Z_2^2+1)^2}\right)\right).$$

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 $t \geq 10$,

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

Therefore, we have verified that the integrand $\log \frac{\phi(R_{n-t,t};ix)}{\phi(P_n^{6,6};ix)}$ is monotonically decreasing in n for $n = 4k$. That is, $E(R_{n-t,t}) - E(P_n^{6,6}) \leq E(R_{10,10}) - E(P_{12}^{6,6}) < 0$ 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 Theorem1.5 is now complete. ∎

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