MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **64** (2010) 61-64

ISSN 0340 - 6253

Note on Bipartite Unicyclic Graphs of Given Bipartition with Minimal Energy*

Jing Li, Xueliang Li

Center for Combinatorics and LPMC-TJKLC

Nankai University, Tianjin 300071, P.R. China

E-mail: `sdlijing1122@163.com; lxl@nankai.edu.cn`

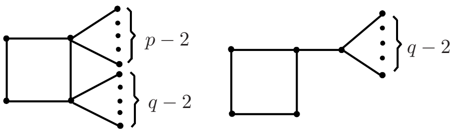
(Received April 16, 2009)

Abstract

The energy of a graph G is defined as the sum of the absolute values of all the eigenvalues of the graph. Let $\mathcal{UB}(p,q)$ denote the set of all bipartite unicyclic graphs of a given (p,q)-bipartition, where $q \geq p \geq 2$. $B(p,q)$ denotes the graph formed by attaching $p-2$ and $q-2$ vertices to two adjacent vertices of a quadrangle C_4, respectively, and $H(3,q)$ denotes the graph formed by attaching $q-2$ vertices to the pendent vertex of $B(2,3)$. In the paper "F. Li and B. Zhou, Minimal energy of bipartite unicyclic graphs of a given bipartition, MATCH Commun. Math. Comput. Chem. 54(2005), 379–388", the authors proved that either $B(3,q)$ or $H(3,q)$ is the graph with minimal energy in $\mathcal{UB}(3,q)(q \geq 3)$. At the end of the paper they conjectured that $H(3,q)$ achieves the minimal energy in $\mathcal{UB}(3,q)$ and checked that this is true for $q=3,4$. However, they could not find a proper way to prove it generally. This short note is to give a confirmative proof to the conjecture.

*Supported by NSFC No.10831001, PCSIRT and the "973" program.

Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of a graph G of order n. The energy of G is defined as $E(G) = |\lambda_1| + |\lambda_2| + \ldots + |\lambda_n|$. For more information on the energy of graphs, we refer to [1]. Let $\mathcal{UB}(p,q)$ denote the set of all bipartite unicyclic graphs of a given (p,q)-bipartition, where $q \geq p \geq 2$. $B(p,q)$ denotes the graph formed by attaching $p-2$ and $q-2$ vertices to two adjacent vertices of a quadrangle C_4, respectively, and $H(3,q)$ denotes the graph formed by attaching $q-2$ vertices to the pendent vertex of $B(2,3)$. See Figure 1 for the graphs $B(p,q)(q \geq p \geq 2)$ and $H(3,q)(q \geq 3)$. For terminology and notations not defined here, we refer to [1, 2] and the references therein.



$B(p,q)$ $H(3,q)$

Figure 1: Graphs $B(p,q)$ $(q \geq p \geq 2)$ and $H(3,q)$ $(q \geq 3)$.

In [2] the authors proved that either $B(3,q)$ or $H(3,q)$ achieves the minimal energy in the class $\mathcal{UB}(3,q)$ of bipartite unicyclic graphs of a $(3,q)$-bipartition $(q \geq 3)$. But, they could not determine which one is smaller. At the end of paper [2] they conjectured that $H(3,q)$ *achieves the minimal energy in* $\mathcal{UB}(3,q)$ and checked that this is true for $q = 3, 4$. However, they could not find a proper way to prove it generally. In this short note we will give a confirmative proof to the conjecture.

Theorem 1 $H(3,q)$ $(q \geq 3)$ *achieves the minimal energy in* $\mathcal{UB}(3,q)$.

Proof. Since from [2] either $B(3,q)$ or $H(3,q)$ achieves the minimal energy in $\mathcal{UB}(3,q)$, we only need to prove that $E(B(3,q)) > E(H(3,q))$.

In fact, for $B(3,q)$ and $H(3,q)$ we have from [2] the characteristic polynomials:

$$\begin{aligned}
\phi(B(3,q)) &= x^{q-3}(x^6 - (q+3)x^4 + (3q-4)x^2 - (q-2)), \\
\phi(H(3,q)) &= x^{q-1}(x^4 - (q+3)x^2 + (4q-6)).
\end{aligned}$$

Suppose that

$$
\begin{aligned}
f(x) &= x^6-(q+3)x^4+(3q-4)x^2-(q-2)\\
&= (x-\sqrt{x}_1)(x-\sqrt{x}_2)(x-\sqrt{x}_3)(x+\sqrt{x}_1)(x+\sqrt{x}_2)(x+\sqrt{x}_3).\\
g(y) &= y^4-(q+3)y^2+(4q-6)\\
&= (x-\sqrt{y}_1)(x-\sqrt{y}_2)(x+\sqrt{y}_1)(x+\sqrt{y}_2).
\end{aligned}
$$

Then, from the relations between the roots and the coefficients of a polynomial equation, we have that $x_1+x_2+x_3=q+3$, $x_1x_2+x_2x_3+x_1x_3=3q-4$ and $x_1x_2x_3=q-2$, and $y_1+y_2=q+3$ and $y_1y_2=4q-6$.

Let $f_0(x)=x^3-(q+3)x^2+(3q-4)x-(q-2)$. It is easy to check that $f_0(0)<0$, $f_0(0.6)>0$, $f_0(q)<0$, $f_0(q^{10})>0$, since $q\geq 3$. Suppose that $x_1\leq x_2\leq x_3$. Then, clearly $x_3>q$ and $\sqrt{x}_1+\sqrt{x}_2+\sqrt{x}_3>\sqrt{x}_3>\sqrt{q}$. So,

$$
\begin{aligned}
& (\sqrt{x_1x_2}+\sqrt{x_2x_3}+\sqrt{x_1x_3})^2\\
=\ & x_1x_2+x_2x_3+x_1x_3+2\sqrt{x_1x_2x_3}(\sqrt{x}_1+\sqrt{x}_2+\sqrt{x}_3)\\
>\ & 3q-4+2\sqrt{q-2}\sqrt{q}>4q-6.
\end{aligned}
$$

Thus,

$$
\begin{aligned}
& (\sqrt{x}_1+\sqrt{x}_2+\sqrt{x}_3)^2\\
=\ & x_1+x_2+x_3+2(\sqrt{x_1x_2}+\sqrt{x_2x_3}+\sqrt{x_1x_3})\\
>\ & q+3+2\sqrt{4q-6}\\
=\ & y_1+y_2+2\sqrt{y_1y_2}\\
=\ & (\sqrt{y}_1+\sqrt{y}_2)^2.
\end{aligned}
$$

Finally, we get that for $q\geq 3$,

$$
E(B(3,q)) = 2(\sqrt{x_1}+\sqrt{x_2}+\sqrt{x_3})>2(\sqrt{y_1}+\sqrt{y_2})=E(H(3,q)).
$$

The theorem is thus proved. ∎

References

[1] I. Gutman, X. Li, J. B. Zhang, Graph Energy, in: M. Dehmer, F. Emmert–Streib (Eds.), *Analysis of Complex Networks: From Biology to Linguistics*, Wiley–VCH Verlag, Weinheim, 2009, pp. 145–174.

[2] F. Li, B. Zhou, Minimal energy of bipartite unicyclic graphs of a given bipartition, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 379–388.