On minimal energy of bipartite unicyclic graphs of a given bipartition

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Abstract

The energy of a graph G, denoted by $E(G)$, is defined to be the sum of absolute values of all eigenvalues of the adjacency matrix of G. Let $\mathscr{B}(p,q)$ denote the set of bipartite unicyclic graphs with a $(p,q)-$bipartition, where $q \geq p \geq 2$. Recently, Li and Zhou [MATCH Commun. Math. Comput. Chem. 54 (2005) 379-388.] conjectured that for $q \geq 3$, $E(B(3,q)) > E(H(3,q))$, where $B(3,q)$ and $H(3,q)$ are respectively graphs as shown in Fig.1. In this note, we show that this conjecture is true for $3 \leq q \leq 217$. As a byproduct, we determined the graph with minimal energy among all graphs in $\mathscr{B}(3,q)$.

Key Words: Bipartite unicyclic graph; Energy of graph; Spectrum of graph; Bipartition.

MSC (2000): 05C35, 05C50, 05C90.

1 Introduction

Given that G is a connected graph with n vertices, and that $A(G)$ is the adjacency matrix of G. The characteristic polynomial $\phi(G;\lambda)$ of $A(G)$ is

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then defined as

$$\phi(G;\lambda) = det(\lambda I - A(G)) = \sum_{i=0}^{n} a_i \lambda^{n-i},$$

where I is the unit matrix of order n.

All n roots $\lambda_1, \lambda_2, \cdots, \lambda_n$ of the equation $\phi(G;\lambda) = 0$ are called to be eigenvalues of G. It's evident that each λ_i $(i = 1, 2, \cdots n)$ is real since $A(G)$ is symmetric.

In chemistry, the (experimentally determined) heats of formation of conjugated hydrocarbons are closely related to total π−electron energy. Within the framework of the so-called HMO model the total π−electron energy is calculated from the eigenvalues of a pertinently constructed molecular graph G by the equation $E(G) = \sum_{i=1}^{n} |\lambda_i|$.

It's well-known that if G is a bipartite graph possessing n vertices, then $\phi(G;x)$ can be expressed as

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

where $b(G,k) \geq 0$ for $k = 0, 1, \cdots, \lfloor \frac{n}{2} \rfloor$. In particular, $b(G,0) = 1$ and $b(G,1)$ equals exactly the number of edges of G.

Based on the expression for $\phi(G;x)$, a quasi-order relation is then introduced over the whole class of bipartite graphs [5]: if G_1 and G_2 are bipartite graphs, then

$$b(G_1,k) \geq b(G_2,k) \ for \ all \ k \geq 0 \Leftrightarrow G_1 \succeq G_2. \qquad (1)$$

If $G_1 \succeq G_2$ and there exists some k_0 such that $b(G_1,k_0) > b(G_2,k_0)$, then we write $G_1 \succ G_2$.

It's long–known that for a bipartite graph G of order n, its energy $E(G)$ can be expressed as the Coulson integral formula (see [3,17])

$$E(G) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} ln \left(\sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} b(G,k) x^{2k} \right) dx. \qquad (2)$$

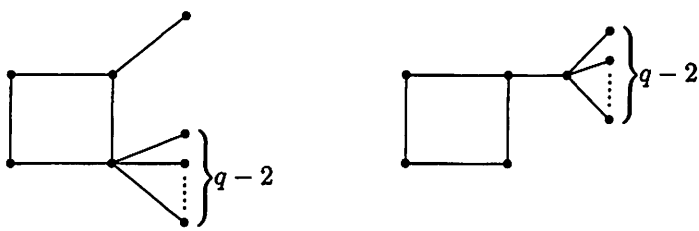
Notice that for any two bipartite graphs G_1 and G_2, $b(G_i,k) \geq 0$ for all $k \geq 0$ and $i = 1, 2$. Then by means of Eq.(2), we have

$$G_1 \succ G_2 \Rightarrow E(G_1) > E(G_2). \qquad (3)$$

A graph is said to be unicyclic if it owns equal number of vertices and edges. Let G be a connected simple graph, if its vertex set V can be partitioned into two parts V_1 and V_2 such that $|V_1| = p$ and $|V_2| = q$, then we call G a graph of a $(p, q)-$bipartition.

It is both interesting and significant to determine the graph with extremal energies among a given class of graphs. Numerous results on this subject have been put forward. For more details see [1–7]; for some recent research along this line see [8–16]. The interested reader may also refer to [17,18] for the mathematical properties on $E(G)$.

Let $\mathscr{B}(p, q)$ denote the set of bipartite unicyclic graphs with a $(p, q)-$bipartition, where $q \geq p \geq 2$. Fig.1 illustrated graphs $B(3, q)$ and $H(3, q)$, respectively.



$(a).B(3, q)$ $(q \geq 3)$ $(b).H(3, q)$ $(q \geq 3)$

Figure 1

Recently, Li and Zhou [11] investigated the minimal energy of bipartite graphs with a given $(p, q)-$bipartition for $q \geq p \geq 2$. They determined the minimal-energy graph among all bipartite unicyclic graphs of a $(p, q)-$bipartition for $q \geq p \geq 4$ or $p = 2$ and $q \geq 2$. When dealing with the minimal energy of bipartite graphs with a given $(3, q)-$bipartition, they posed the following conjecture:

Conjecture. *For all* $q \geq 3$, $E(B(3, q)) > E(H(3, q))$.

In this note, we shall prove that this conjecture is true for $3 \leq q \leq 217$.

2 The proof of conjecture for the case $3 \leq q \leq 217$

By a direct calculation, one can easily obtain

$$\phi(B(3,q);x) = x^{q-3}\left[x^6 - (q+3)x^4 + (3q-4)x^2 - (q-2)\right], \quad (4)$$

$$\phi(H(3,q);x) = x^{q-1}\left[x^4 - (q+3)x^2 + (4q-6)\right]. \quad (5)$$

From the above two equalities it is concluded that neither $H(3,q) \not\prec B(3,q)$ nor $B(3,q) \not\succ H(3,q)$. Moreover, even if we use the Coulson integral formula (see Eq.(2)), we still can not determine which of two graphs $B(3,q)$ and $H(3,q)$ has smaller energy.

Now, we shall use one famous result introduced in spectral graph theory [19]. It is well known that the eigenvalues of a graph G are not mutually independent, and there exist some relations between them. One of such relations between eigenvalues holding for a bipartite graph is the pairing theorem [19]:

$$\lambda_i - \lambda_{n+1-i} = 0 \text{ for } i = 1,\, 2,\, \cdots,\, n. \quad (6)$$

Now we can state and prove the following:

Theorem 1 *Let* $3 \leq q \leq 217$, *then* $E(B(3,q)) > E(H(3,q))$.

Proof. It is evident that both $H(3,q)$ and $B(3,q)$ are all bipartite graphs. Suppose that $a_1 \geq a_2 \geq a_3 > 0$ and $a_4 \geq a_5 > 0$. Then by means of Eqs.(4)–(6), we may assume that the non-zero eigenvalues of $B(3,q)$ and $H(3,q)$ are respectively $\pm\sqrt{a_1}, \pm\sqrt{a_2}, \pm\sqrt{a_3}$ and $\pm\sqrt{a_4}, \pm\sqrt{a_5}$. Thus we can rewrite the respective characteristic polynomials of $B(3,q)$ and $H(3,q)$ as follows:

$$\phi(B(3,q);x) = x^{q-3}(x^2 - a_1)(x^2 - a_2)(x^2 - a_3), \quad (7)$$

$$\phi(H(3,q);x) = x^{q-1}(x^2 - a_4)(x^2 - a_5). \quad (8)$$

Note that the zero-eigenvalues play no role in computing the energy $E(G)$ for a graph G. Then we have $E(B(3,q)) = 2(\sqrt{a_1}+\sqrt{a_2}+\sqrt{a_3})$ and $E(H(3,q)) = 2(\sqrt{a_4}+\sqrt{a_5})$.

Now, equating Eq.(4) and Eq.(7) and comparing the coefficients deduce that

$$\begin{cases} a_1 + a_2 + a_3 = q + 3 \\ a_1a_2 + a_2a_3 + a_3a_1 = 3q - 4 \\ a_1a_2a_3 = q - 2 \end{cases}.$$

Similarly, we have

$$\begin{cases} a_4 + a_5 = q + 3 \\ a_4a_5 = 4q - 6 \end{cases}.$$

Next, we shall verify that $E(S_{p+5}^{4,p}) > E(R_{p+5}^{4,p})$, or equivalently, prove that

$$\sqrt{a_1} + \sqrt{a_2} + \sqrt{a_3} > \sqrt{a_4} + \sqrt{a_5}.$$

That is,

$$(a_1 + a_2 + a_3) + 2(\sqrt{a_1a_2} + \sqrt{a_2a_3} + \sqrt{a_3a_1}) > (a_4 + a_5) + 2\sqrt{a_4a_5},$$

i.e.,

$$\sqrt{a_1a_2} + \sqrt{a_2a_3} + \sqrt{a_3a_1} > \sqrt{a_4a_5},$$

i.e.,

$$(a_1a_2 + a_2a_3 + a_3a_1) + 2\sqrt{a_1a_2a_3}(\sqrt{a_1} + \sqrt{a_2} + \sqrt{a_3}) > a_4a_5,$$

i.e.,

$$3q - 4 + 2\sqrt{q-2}(\sqrt{a_1} + \sqrt{a_2} + \sqrt{a_3}) > 4q - 6,$$

i.e.,

$$\sqrt{a_1} + \sqrt{a_2} + \sqrt{a_3} > \frac{\sqrt{q-2}}{2}.$$

Recall that

$$\sqrt{a_1}+\sqrt{a_2}+\sqrt{a_3} = \sqrt{\frac{a_1a_2a_3}{a_2a_3}}+\sqrt{a_2}+\sqrt{a_3} = \sqrt{\frac{q-2}{a_2a_3}}+\sqrt{a_2}+\sqrt{a_3} \geq 3\sqrt[6]{q-2}.$$

So it suffices to prove that

$$3\sqrt[6]{q-2} > \frac{\sqrt{q-2}}{2},$$

i.e,

$$(q-2)^2 < 6^6,$$

which gives $q < 218$. This completes the proof.

Li and Zhou [11] obtained the following result.

Lemma 2 *Let* $G \in \mathscr{B}(3,q)$*. If* $G \ncong B(3,q)$, $H(3,q)$*, then* $E(G) > E(B(3,q))$.

Combining Theorem 1 and Lemma 2, we obtain

Corollary 3 *Let* $G \in \mathscr{B}(3,q)$ *with* $3 \leq q \leq 217$*. If* $G \ncong H(3,q)$*, then* $E(G) > E(H(3,q))$.

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