On bipartite graphs with minimal energy *

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Abstract

The energy of a graph is the sum of the absolute values of the eigenvalues of the graph. In a paper *"J. Chem. Inf. Comput. Sci. 39(1999), 984–996"* Caporossi et al. conjectured that among all connected graphs G with $n \geq 6$ vertices and $n-1 \leq m \leq 2(n-2)$ edges, the graphs with minimum energy are the star S_n with $m-n+1$ additional edges all connected to the same vertices for $m \leq n+\lfloor (n-7)/2 \rfloor$, and the bipartite graph with two vertices on one side, one of which is connected to all vertices on the other side otherwise. The conjecture is proved to be true for $m = n-1,\ 2(n-2)$ in the same paper by Caporossi et al. themselves, and $m = n$ by Hou in "J. Math. Chem. 29(2001), 163–168". In this paper, we give a complete solution to the second part of the conjecture on bipartite graphs. Moreover, we determine the graph with the second-minimal energy in all connected bipartite graphs with n vertices and $m\,(n \leq m \leq 2n-5)$ edges.

Keywords: Minimal energy, Characteristic polynomial, Eigenvalue, Bipartite graph

AMS Subject Classification 2000: 05C35; 05C50; 05C90

1 Introduction

Let $G = (V, E)$ be a graph without loops or multiple edges with vertex set $V = \{v_1, v_2, \ldots, v_n\}$ and edge set E. Denote the degree of vertex v_i by $d(v_i)$. The adjacency matrix $A(G) = [a_{ij}]$ of G is an $n \times n$ symmetric matrix of 0's and l's with $a_{ij} = 1$ if and only if v_i and v_j are joined by an edge.

*Supported by CityU Project No.7001996, PCSIRT, NSFC and the "973" program

We denote by $\phi(G,x)$ the characteristic polynomial $\det(xI - A(G))$ of G and call the roots of $\det(xI - A(G)$ the eigenvalues of G. It is well known [3] that if G is a bipartite graph, then

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

where $b_{2i}(G) = (-1)^i a_{2i}$ and $b_{2i}(G) \geq 0$ for all $i = 1, \ldots, \lfloor \frac{n}{2} \rfloor$. Clearly, $b_0(G) = 1$ and $b_2(G)$ equals the number of edges of G.

In chemistry, the experimental heats from the formation of conjugated hydrocarbons are closely related to the total π-electron energy. And the calculation of the total energy of all π-electrons in conjugated hydrocarbons can be reduced to (within the framework of HMO approximation) [6] that of

$$E = E(G) = \sum_{i=0}^{n} |\lambda_i|, \tag{1}$$

where λ_i are the eigenvalues of the corresponding graph G. The right-hand side of Eq.(1) is defined for all graphs (no matter whether they represent the carbon-atom skeleton of a conjugated electron system or not). In view of this, if G is any graph, then by means of Eq.(1) one defines $E(G)$ and calls it the energy of the graph G. Recently, it has been intensively studied by some researchers (See [1, 4, 7, 8, 9, 10, 11, 14, 15, 12, 13, 17]). For a survey of the mathematical properties and results on $E(G)$, see the recent review paper [5].

It is known [6] that for bipartite graph G, $E(G)$ can be also expressed as the Coulson integral formula

$$E(G) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \ln \left[1 + \sum_{i=0}^{\lfloor n/2 \rfloor} b_{2i} x^{2i} \right] dx. \tag{2}$$

If for two bipartite graphs G_1 and G_2, $b_{2i}(G_1) \leq b_{2i}(G_2)$ holds for all $i = 1, 2, \ldots, \lfloor n/2 \rfloor$, we say that G_1 is smaller than G_2, and write $G_1 \preceq G_2$ or $G_2 \succeq G_1$. Moreover, if $b_{2i}(G_1) < b_{2i}(G_2)$ holds for some i, we write $G_1 \prec G_2$ or $G_2 \succ G_1$. From Eq.(2) we know that for two bipartite graphs G_1 and G_2

$$G_1 \preceq G_2 \Rightarrow E(G_1) \leq E(G_2)$$
$$G_1 \prec G_2 \Rightarrow E(G_1) < E(G_2)$$

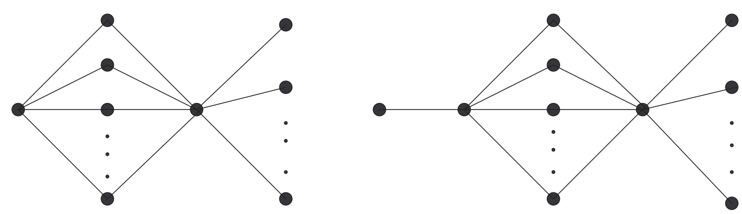
If a graph G has n vertices, then we say that G is an n-graph; if G has n vertices and m edges, then G is called an (n, m)-graph. Many results on the minimal energy have been obtained for various classes of graphs. In [1], Caporossi et al. gave the following conjecture.

Conjecture 1 *Among all connected graphs G with $n \geq 6$ vertices and $n-1 \leq m \leq 2(n-2)$ edges, the graphs with minimum energy are the star S_n with $m-n+1$ additional edges all connected to the same vertices for $m \leq n + \lfloor (n-7)/2 \rfloor$, and the bipartite graph with two vertices on one side, one of which is connected to all vertices on the other side otherwise.*

This conjecture is proved to be true for $m = n-1,\ 2(n-2)$ [1, Theorem 1], and $m = n$ [9].

The main purpose of this paper is to consider connected bipartite graphs. Clearly, the extremal bipartite graphs of Conjecture 1 is a connected (n,m)-graph such that $n \leq m \leq 2(n-2)$.

Let $B_{n,m}$ be the bipartite (n,m)-graph with two vertices on one side, one of which is connected to all vertices on the other side otherwise. Let $B'_{n,m}$ be the graph obtain from $B_{n-1,m-1}$ by adding a pendant edge to the vertex of second maximal degree in $B_{n-1,m-1}$ (see Figure 1).



$B_{n,m}$ $B'_{n,m}$

Figure 1: Graphs $B_{n,m}$ and $B'_{n,m}$.

In this paper, we will show that $B_{n,m}$ is the unique graph with minimal energy in all bipartite connected (n,m)-graphs for $n \leq m \leq 2(n-2)$, giving a complete solution to the above Conjecture 1 on bipartite graphs. Moreover, we prove that $B'_{n,m}$ is the unique graph with second-minimal energy in all bipartite connected (n,m)-graphs for $n \leq m \leq 2n-5$.

2 Main result

Let G be a graph with characteristic polynomial $\phi(G,\lambda) = \sum_{i=0}^{n} a_i \lambda^{n-i}$. Then for $i \geq 1$

$$a_i = \sum_{S \in L_i} (-1)^{p(S)} 2^{c(S)},$$

where L_i denotes the set of Sachs' subgraphs (see [3]) of G with i vertices, that is, the graphs S in which every component is either a K_2 or a cycle, $p(S)$

is the number of components of S and $c(S)$ is the number of cycles contained in S. In addition, $a_0 = 1$.

By Sachs' Theorem [3] we have

Lemma 1 *[18]* $b_4(G) = m(G, 2) - 2q(G)$, *where* $q(G)$ *denotes the number of quadrangles in* G.

Lemma 2 *Let* uv *be a cut edge in* G. *Then*

$$b_4(G) = b_4(G - uv) + e(G - u - v).$$

In particular, let uv *be a pendant edge of* G *with the pendant vertex* v, *then*

$$b_4(G) = b_4(G - v) + e(G - u - v).$$

Proof. Since uv is a cut edge, we have $q(G) = q(G - uv)$. By Lemma 1 we have

$$\begin{aligned} b_4(G - uv) &= m(G - uv, 2) - 2q(G - uv), \\ b_4(G) &= m(G, 2) - 2q(G) \\ &= m(G - uv, 2) + m(G - u - v, 1) - 2q(G) \\ &= b_4(G - uv) + e(G - u - v). \end{aligned}$$

We thus obtain the result. □

Theorem 1 $B_{n,m}$ $(n \leq m \leq 2(n-2))$ *is the unique graph with minimal energy in all bipartite connected* (n, m)*-graphs.*

Proof. Let G be a bipartite connected (n, m)-graph. Then $\Delta(G) \leq n - 2$.

Since $b_i(B_{n,m}) = 0$ for $i \neq 0, 2, 4$, we have that $b_0(G) = 1$ and $b_2(G) = m$. It suffices to prove that $b_4(G) \geq b_4(B_{n,m})$. We apply induction on n to prove it. From the table of [2] the result is true for $n = 7$. So we suppose that $n \geq 8$ and the result is true for smaller n.

Case 1. There is a pendant edge uv in G with pendant vertex v. Then, by Lemma 2 we have

$$b_4(G) = b_4(G - v) + e(G - u - v).$$

Since $\Delta(G) \leq n - 2$, we have $e(G - u - v) \geq m - \Delta(G) \geq m - n + 2 = e(S_{m-n+3})$. By induction hypothesis, $b_4(G - v) \geq b_4(B_{n-1,m-1})$. Since $b_4(B_{n,m}) = b_4(B_{n-1,m-1}) + e(S_{m-n+3})$, we get the result $b_4(G) \geq b_4(B_{n,m})$.

Case 2. There are no pendant vertices in G.

Claim 1. Let G be a connected bipartite (n,m)-graph for $n \leq m \leq 2(n-2)$. Then $q(G) \leq \binom{m-n+2}{2}$, where $q(G)$ denotes the number of quadrangles in G.

Proof. We apply induction on m. The result is obvious for $m = n$. So we suppose $n \leq m \leq 2(n-2)$ and the result is true for smaller m.

Let e be an edge of a cycle in G. Then G contains at most $m-n+1$ quadrangles containing the edge e. Otherwise, we suppose that there are $m-n+a\,(a \geq 2)$ quadrangles containing $e = uv$. Let U be a set of neighbor vertices of u except v, and let V be a set of neighbor vertices of v except u. Then there are just $m-n+a$ edges between U and V. Let X be a subset of U such that each vertex in X is incident to some of the above $m-n+a$ edges and Y be a subset of V defined similarly to X. Assume $|X| = x, |Y| = y$. Let G_0 be a subgraph of G induced by $V(G_0) = u \cup v \cup X \cup Y$. There are at least $m-n+a+x+y+1$ edges and exactly $x+y+2$ vertices in G_0. In order to make the remaining vertices connect to G_0, the number of remaining edges is not less than that of remaining vertices:

$$m - (m-n+a+x+y+1) \geq n - (x+y+2), \tag{3}$$

that is,

$$n - a - 1 \geq n - 2\,(a \geq 2).$$

This is an contradiction. Note that Ineq.(3) still holds when there is no remaining vertices.

Let $q_G(e)$ denotes the number of quadrangles in G. Thus we have

$$\begin{aligned} q(G) &= q_G(e) + q(G-e) \\ &\leq m-n+1+\tbinom{m-1-n+2}{2} = \tbinom{m-n+2}{2}, \end{aligned}$$

where $q(G-e) \leq \binom{m-1-n+2}{2}$, obtained by the induction hypothesis. $\square$

A nonincreasing sequence $(d)_G = (d_1, d_2, \ldots, d_n)$ of positive integers is said to be graphic if there a simple graph G having degree sequence $(d)_G$.

Claim 2. Let G be a bipartite connected (n,m)-graph. If G has no pendant vertices, then

$$\sum_{v \in V(B_{n,m})} \binom{d(v)}{2} \geq \sum_{v \in V(G)} \binom{d(v)}{2}.$$

Proof. Let

$$(d)_G = (d_1, d_2, \dots d_{i-1}, d_i, \dots, d_j, d_{j+1}, \dots, d_n),$$

and

$$(d)' = (d_1, d_2, \dots d_i, d_i + 1, \dots, d_j - 1, d_{j+1}, \dots, d_n).$$

where $d_i \geq d_j$. By writing

$$(d)' = (d'_1, d'_2, \dots d'_{i-1}, d'_i, \dots, d'_j, d'_{j+1}, \dots, d'_n),$$

we can obtain that $\sum\limits_{t=1}^{n} \binom{d'_t}{2} > \sum\limits_{t=1}^{n} \binom{d_t}{2}$, since

$$\sum_{t=1}^{n} \binom{d'_t}{2} - \sum_{t=1}^{n} \binom{d_t}{2} = \binom{d_i+1}{2} + \binom{d_j-1}{2} - \left(\binom{d_i}{2} + \binom{d_j}{2}\right) = d_i - d_j + 2 > 0.$$

Notice that $d_1 \geq d_2 \geq \cdots \geq d_n \geq 2$ and $d_1 + d_2 + \cdots + d_n = 2m$. Repeating this procession, we can obtain the sequence

$$(d'') = (d''_1, d''_2, d_3, \dots, d_{m-n+4}, \overbrace{1, 1, \dots, 1}^{2n-m-4}).$$

where $d''_1 \leq n-2$, $d''_2 \geq d_2$ if $d''_1 = n-2$, and $d''_2 = d_2$ if $d''_1 < n-2$. Since $d''_1 \geq d''_2 \geq d_3 \geq \cdots \geq d_{m-n+4} \geq 2$, by applying the above procession repeatedly we finally obtain the degree sequence $(d)_{B_{n,m}}$:

$$(d)_{B_{n,m}} = (n-2, m-n+2, \overbrace{2, 2, \dots, 2}^{m-n+2}, \overbrace{1, 1, \dots, 1}^{2n-m-4}),$$

which has the maximum value of $\sum_{v \in V(G)} \binom{d(v)}{2}$. The proof of the claim is thus complete. $\square$

For a simple graph G, we have $m(G, 2) = \binom{m}{2} - \sum_{v \in V(G)} \binom{d(v)}{2}$. By Lemma 1 we know that

$$b_4(G) = \binom{m}{2} - \sum_{v \in V(G)} \binom{d(v)}{2} - 2q(G).$$

By Claims 1 and 2, we can easy obtain the result.

Combining all the above cases we thus complete the proof. $\square$

Since the characteristic polynomial of $B_{n,m}$ is

$$\phi(B_{n,m}, x) = x^{n-4}[x^4 - mx^2 + (m-n+2)(2n-m-4)],$$

by simple computation we have

Corollary 1 *Let G be a bipartite connected (n,m)-graph with $n \leq m \leq 2n-4$. Then*

$$E(G) \;\geq\; 2\sqrt{m+2\sqrt{(m-n+2)(2n-m-4)}},$$

with equality if and only if $G \cong B_{n,m}$.

Theorem 2 *$B'_{n,m}$ $(n \leq m \leq 2n-5)$ is the unique graph with second minimal energy in all bipartite connected (n,m)-graphs.*

Proof. Since $b_0(B'_{n,m}) = 1, b_2(B'_{n,m}) = m, b_4(B'_{n,m}) = (m-n+3)(2n-m-4)-1$ and $b_i(B'_{n,m}) = 0$ for other positive integer i, similar to the proof of Theorem 1 we can obtain the result. $\square$

Analogously, we have

$$\phi(B'_{n,m}, x) = x^{n-4}\{x^4 - mx^2 + [(m-n+3)(2n-m-4)-1]\},$$

and therefore

Corollary 2 *Let G be a bipartite connected (n,m)-graph with $n \leq m \leq 2n-5$. If $G \ncong B_{n,m}$, then*

$$E(G) \;\geq\; 2\sqrt{m+2\sqrt{(m-n+3)(2n-m-4)-1}},$$

with equality if and only if $G \cong B'_{n,m}$.

References

[1] G. Caporossi, D. Cvetković, I. Gutman and P. Hansen, Variable neighborhood search for extremal graphs. 2. Finding graphs with external energy, J. Chem. Inf. Comput. Sci. 39(1999), 984–996.

[2] D. Cvetković, M. Doob, I. Gutman and A. Torĝasev, *Recent results in the theory of graph spectra*, North-Holland, Amsterdam, 1988.

[3] D. Cvetković, M. Doob and H. Sachs, *Spectra of Graphs–Theory and Applications*, Academic Press, New York, 1980.

[4] I. Gutman, Acyclic systems with extremal Hückel π-electron energy, Theoret. Chim. Acta (Berlin) 45(1977), 79–87.

[5] I. Gutman, The energy of a graph: old and new results, in: *Algebraic Combinatorics and Applications*, eds. A. Betten, A. Kohnert, R. Laue and A. Wassermann (Springer-Verlag, Berlin, 2001), pp. 196–211.

[6] I. Gutman and O.E. Polansky, *Mathematicl Concepts in Organic Chemistry*, Springer-Verlag, Berlin, 1986.

[7] I. Gutman, B. Zhou, Laplacian energy of a graph, Linear Algebra Appl. 414(2006) 29C37.

[8] W. Haemers, Strongly regular graphs with maximal energy, Linear Algebra Appl., in press.

[9] Y. Hou, Unicyclic graphs with minimal energy, J. Math. Chem. 29(2001), 163–168.

[10] J. Koolen and V. Moulton, Maximal energy graphs, Adv. Applied Math. 26(2001), 47-52.

[11] J. Koolen and V. Moulton, Maximal energy bipartite graphs, Graphs Combin. 19(2003), 131-135.

[12] X. Li and J. Zhang, On bicyclic graphs with maximal energy. Linear Algebra Appl. 427 (2007), 87-98.

[13] X. Li, J. Zhang and B. Zhou, On unicyclic conjugated molecules with minimal energies, J. Math. Chem. 42(2007) 729-740.

[14] V. Nikiforov, Graphs and matrices with maximal energy, J. Math. Anal. Appl. 327(2007), 735-738.

[15] J. Rada and A. Tineo, Upper and lower bounds for the energy of bipartite graphs, J. Math. Anal. Appl. 289(2004), 446-455.

[16] J. Rada, Energy ordering of catacondensed hexagonal systems, Discete Appl. Math. 145(2005) 437-443.

[17] F. Zhang and H. Li, On acyclic conjugated molecules with minimal energies, Discete Appl. Math. 92(1999) 71-84.

[18] J. Zhang and B. Zhou, On bicyclic graphs with minimal energies, J. Math. Chem. 37(4)(2005), 423–431.