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Unicyclic graphs with minimal energy *

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If G is a graph and $\lambda_1, \lambda_2, \ldots, \lambda_n$ are its eigenvalues, then the energy of G is defined as $E(G) = |\lambda_1| + |\lambda_2| + \cdots + |\lambda_n|$. Let S_n^3 be the graph obtained from the star graph with n vertices by adding an edge. In this paper we prove that S_n^3 is the unique minimal energy graph among all unicyclic graphs with n vertices ($n \geqslant 6$).

KEY WORDS: unicyclic graph, energy of graph, spectra of graph

1. Introduction

Let G be a graph with n vertices and $A(G)$ the adjacency matrix of G. The characteristic polynomial of $A(G)$

$$\phi(G; x) = \det\bigl(xI - A(G)\bigr) = \sum_{i=0}^{n} a_i x^{n-i}, \tag{1}$$

where I stands for the unit matrix of order n, is called to be the characteristic polynomial of the graph G. The n roots of the equation $\phi(G; x) = 0$, denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$, are called to be the eigenvalues of the graph G. Since $A(G)$ is symmetric, all eigenvalues of $A(G)$ are real.

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) (see [1]) that

$$E(G) = \sum_{i=1}^{n} |\lambda_i|, \tag{2}$$

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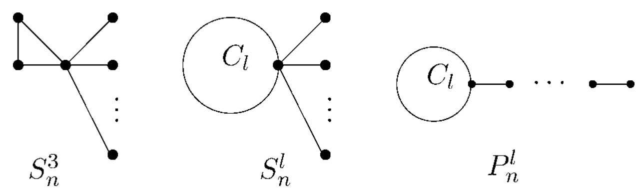

Figure 1.

where $\lambda_1, \ldots, \lambda_n$, are all eigenvalues of the corresponding molecular graph G. $E(G)$ can be expressed as the Coulson integral formula (see [1])

$$E(G) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \frac{1}{x^2} \ln\left[\left(\sum_{j=0}^{\lceil n/2\rceil}(-1)^j a_{2j}x^{2j}\right)^2 + \left(\sum_{j=0}^{\lceil n/2\rceil}(-1)^j a_{2j+1}x^{2j+1}\right)^2\right]\mathrm{d}x, \quad (3)$$

where $a_0, a_1, \ldots, a_n$ are the coefficients of the characteristic polynomial of G.

The right-hand side of equation (2) is defined for all graphs (no matter whether they are molecular graphs or not). In view of this, if G is any graph, then by means of equation (2) one defines $E(G)$ and calls it *the energy of the graph G*. For a survey of the mathematical properties of $E(G)$ see [1, chapter 12] and the review [2].

There are a lot of results on the bounds for $E(G)$ which pertain to special types of graphs: bipartite, benzenoid, trees (see [2–6]). However, up to now, very little is known for graphs with extremal energy. Graphs with extremal energy have been determined only for n-vertex trees (see [3]) and n-vertex trees with perfect matchings (see [7]). Recently, Caporossi et al. [8] have posed the following conjecture, based upon results attained with the computer system AutoGraphix (see [5]).

Conjecture. *Connected graphs G with $n \geqslant 6$ vertices, $n-1 \leqslant e \leqslant 2(n-2)$ edges and minimum energy are stars with $e-n+1$ additional edges all connected to the same vertex for $e \leqslant n + \lfloor (n-7)/2 \rfloor$, and bipartite graphs with two vertices on one side, one of which is connected to all vertices on the other side otherwise.*

This conjecture is true when $e = n-1$ and $e = 2(n-2)$. In this paper we prove the above conjecture is true for $e = n$, that is, amongst all unicyclic graphs with n vertices and n edges, the graph S_n^3 has the minimum energy, where S_n^3 denotes the graph obtained from the star graph with n vertices by adding an edge (see figure 1).

2. Results

In this paper we consider only connected simple graph, and denote by S_n, C_n and P_n the star graph, the cycle graph, and the path graph with n vertices, respectively. Let $G(n,l)$ be the set of all unicyclic graphs with n vertices and with a cycle C_l. Let G be a graph with n vertices, and the characteristic polynomial of G be (1). Set $b_i(G) = |a_i(G)|$, $i = 0, 1, \ldots, n$. Notice that $b_0(G) = 1$, and $b_2(G)$ is the number of edges of G. Let the number of k-matchings of a graph G be $m(G, k)$. If G is acyclic, then $b_{2k} = m(G, k)$ and $b_{2k+1} = 0$ for $k \geqslant 0$.

We recall the Sachs theorem for the coefficients of the characteristic polynomial of a graph (see [9]), that is,

$$a_i = a_i(G) = \sum_{S \in \mathcal{L}_i} (-1)^{k(S)} 2^{c(S)},$$

where $\mathcal{L}_i$ denotes the set of Sachs graphs of G with i vertices, $k(S)$ is the number of components of S and $c(S)$ is the number of cycles contained in S.

Our starting point is the following lemma.

Lemma 1. *Let $G \in G(n, l)$. Then $(-1)^k a_{2k} \geqslant 0$ for all $k \geqslant 0$; and $(-1)^k a_{2k+1} \geqslant 0$ (respectively $\leqslant 0$) for all $k \geqslant 0$ if $l = 2r + 1$ and r is odd (respectively even).*

Proof. If l is even, then G is bipartite, and $a_{2k} = (-1)^k b_{2k}$, $a_{2k+1} = 0$ for all $k \geqslant 0$. Hence the result follows.

Suppose l is odd and $l = 2r + 1$. If $i = 2k$, then every Sachs graph of G with i vertices must consist of only k-matchings, and $a_{2k} = (-1)^k m(G; k)$. If $i = 2k + 1$, then $a_{2k+1} = 0$ when $2k + 1 < l$; and every Sachs graph of G with $2k + 1$ vertices must contain the cycle C_l when $2k + 1 \geqslant l$, thus $a_{2k+1} = 2(-1)^{k-r+1} m(G - C_l, k - r)$. Hence the result follows. □

From equation (3) we have

$$E(G) = \frac{1}{\pi} \int_0^{+\infty} \frac{1}{x^2} \ln\left[\left(\sum_{j=0}^{\lceil n/2 \rceil} b_{2j} x^{2j}\right)^2 + \left(\sum_{j=0}^{\lceil n/2 \rceil} b_{2j+1} x^{2j+1}\right)^2\right] \mathrm{d}x, \tag{4}$$

and it follows that $E(G)$ is a monotonically increasing function of $b_i(G)$, $i = 1, 2, \ldots, n$, that is, let G_1 and G_2 be unicyclic graphs, if

$$b_i(G_1) \geqslant b_i(G_2) \tag{5}$$

holds for all $i \geqslant 0$, then

$$E(G_1) \geqslant E(G_2), \tag{6}$$

and equality in (6) is reached only if (5) is an equality for all $i \geqslant 0$.

If (5) holds for all i, then we will write $G_1 \geqslant G_2$ or $G_2 \leqslant G_1$, and we write $G_1 > G_2$ if $G_1 \geqslant G_2$ but not $G_2 \geqslant G_1$. In terms of this notation, we summarize the above result in a lemma given below.

Lemma 2. *Let G and H be two unicyclic graphs. Then $G \geqslant H$ implies $E(G) \geqslant E(H)$, and $G > H$ implies $E(G) > E(H)$.*

Lemma 3. *Let $G \in G(n, l)$, and edge uv be a pendant edge of G with pendant vertex v. Then*

$$b_i(G) = b_i(G - v) + b_{i-2}(G - v - u). \tag{7}$$

Proof. Since v is a pendant vertex of G, we have

$$\phi(G; x) = x\phi(G - v; x) - \phi(G - v - u; x).$$

Thus

$$\begin{aligned} b_i(G) = \left|a_i(G)\right| &= \left|a_i(G - v) - a_{i-2}(G - v - u)\right| \\ &= \left|a_i(G - v)\right| + \left|a_{i-2}(G - v - u)\right| \\ &= b_i(G - v) + b_{i-2}(G - v - u). \end{aligned}$$ □

Let S_n^l denote the graph obtained from the cycle C_l by adding $n - l$ pendant edges to a vertex of C_l (see figure 1).

Theorem 4. *Let $G \in G(n, l)$, and $G \neq S_n^l$. Then $G > S_n^l$.*

Proof. We prove the theorem by induction on $n - l$.

If $n - l = 0$, then the theorem clearly follows. Let $p \geqslant 1$ and suppose the result is true for $n - l < p$. Now we consider $n - l = p$. Since G is unicyclic and $n > l$, G is not a cycle. Hence G must have a pendant vertex v, and v is adjacent to a unique vertex u. By lemma 3, we have

$$\begin{aligned} b_i(G) &= b_i(G - v) + b_{i-2}(G - v - u), \\ b_i\left(S_n^l\right) &= b_i\left(S_{n-1}^l\right) + b_{i-2}(P_{l-1}). \end{aligned}$$

By the induction assumption, we have

$$b_i(G - v) \geqslant b_i\left(S_{n-1}^l\right) \quad \text{for all } i \geqslant 0. \tag{8}$$

As

$$b_{i-2}(P_{l-1}) = \begin{cases} 0, & \text{if } i \text{ is odd;} \\ m\left(P_{l-1}, \dfrac{i-2}{2}\right), & \text{if } i \text{ is even and } i \leqslant l+1; \\ 0, & \text{if } i \text{ is even and } i > l+1, \end{cases}$$

and $G - v - u$ contains the path P_{l-1} as its subgraph, $b_{i-2}(G - v - u) \geqslant b_{i-2}(P_{l-1})$ if i is odd, or if i is even and $i > l+1$. If i is even and $i \leqslant l+1$, then $b_{i-2}(G - v - u) = m(G - v - u, (i-2)/2) \geqslant m(P_{l-1}, (i-2)/2)$. Thus we have

$$b_{i-2}(G - v - u) \geqslant b_{i-2}(P_{l-1}) \quad \text{for all } i \geqslant 0. \tag{9}$$

From (8) and (9), we have

$$b_i(G) \geqslant b_i\left(S_n^l\right).$$

It is easy to see that if $G \neq S_n^l$ then $b_2(G - v - u) > l - 2 = b_2(P_{l-1})$. Hence $b_4(S_n^l) < b_4(G)$, and the theorem holds. □

Theorem 5. *Let $n \geqslant l \geqslant 5$. Then $S_n^4 < S_n^l$.*

Proof. We prove the theorem by induction on $n - l$. It is easy to obtain that

$$\phi\left(S_n^4; x\right) = x^{n-4}\left[x^4 - nx^2 + 2(n-4)\right]. \tag{10}$$

Thus $b_4(S_n^4) = 2(n-4)$, and $b_i(G) = 0$ for all $i \neq 0, 2, 4$. If $n - l = 0$, then $G = C_n$, and $b_4(C_n) = n/2(n-3)$. Hence $b_4(C_n) > b_4(S_n^4)$ for all $n \geqslant 5$ and the theorem holds. Let $p \geqslant 1$ and suppose the result is true for $n - l < p$. Now we consider $n - l = p$. By lemma 3, we have

$$b_4\left(S_n^l\right) = b_4\left(S_{n-1}^l\right) + b_2(P_{l-1}) = b_4\left(S_{n-1}^l\right) + l - 2 \geqslant 2(n-1-4) + l - 2 > 2(n-4).$$

Thus the theorem follows. □

Theorem 6. *Let G be a unicyclic graph with $n \geqslant 6$ vertices, and $G \neq S_n^3$. Then $E(S_n^3) < E(G)$.*

Proof. From theorems 4 and 5, it is sufficient to prove that $E(S_n^3) < E(S_n^4)$ for $n \geqslant 6$. It is easy to obtain

$$\phi\left(S_n^3; x\right) = x^{n-4}\left[x^4 - nx^2 - 2x + (n-3)\right]. \tag{11}$$

By (4), then we have

$$E\left(S_n^4\right) - E\left(S_n^3\right) = \frac{1}{\pi}\int_0^{+\infty} \frac{1}{x^2} \ln \frac{[1 + nx^2 + 2(n-4)x^4]^2}{[1 + nx^2 + (n-3)x^4]^2 + (2x^3)^2} \mathrm{d}x.$$

Set $f(x) = [1 + nx^2 + 2(n-4)x^4]^2 - [1 + nx^2 + (n-3)x^4]^2 - 4x^6$. Then $f(x) = 2(n-5)x^4 + 2[n(n-5) - 2]x^6 + (n-5)^2x^8 + 2(n-5)(n-3)x^8 > 0$ for $n \geqslant 6$. Therefore, $E(S_n^3) < E(S_n^4)$ for $n \geqslant 6$. □

3. Discussion

The problem of finding unicyclic graphs with maximum energy is more difficult than finding unicyclic graphs with minimum energy. Let P_n^l be the unicyclic graph obtained by connecting a vertex (called the joint point of P_n^l) of the cycle C_l with a terminal vertex of the path P_{n-l} (see figure 1). If l is odd, or $l = 4r + 2$, then, similar to theorem 4, we can prove that, P_n^l has the greatest energy in $G(n, l)$, but in the case of $l = 4r$, we do not know which graph has the greatest energy in $G(n, l)$. It is more interesting that the following conjecture was raised in [8], and is in good agreement with the empirically known facts in chemistry.

Conjecture. *Among unicyclic graphs on n vertices the cycle C_n has maximal energy if $n \leqslant 7$ and $n = 9, 10, 11, 13$ and 15. For all other values of n the unicyclic graph with maximum energy is P_n^6.*

Progress on the above conjecture may refer [10].

Remark. In view of M. Randic (privative communication), the invariant $E(G)$ in formula (2) be better refered to as “graph potency" instead of “graph energy" as initially proposed by I. Gutman. Nevertheless, in this paper we still called $E(G)$ the energy of graph G as before.

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