MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **61** (2009) 479-486

ISSN 0340 - 6253

On Hypoenergetic Unicyclic and Bicyclic Graphs

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(Received June 27, 2008)

Abstract

The energy $E(G)$ of a graph G is the sum of the absolute values of the eigenvalues of G. An n-vertex graph G is said to be hypoenergetic if $E(G) < n$. In [1], I. Gutman et al. showed that: (a) if $\Delta = 3$, then there exist hypoenergetic trees for $n = 4$ and $n = 7$; (b) if $\Delta = 4$, then there exist hypoenergetic trees for all $n \geq 5$ such that $n \equiv k$ $(mod\ 4)$, $k = 0, 1, 3$; (c) if $\Delta \geq 5$, then there exist hypoenergetic trees for all $n \geq \Delta + 1$. In this paper we prove that there exist hypoenergetic unicyclic graphs for all $n \geq 7$ and bicyclic graphs for $n \geq 8$. Moreover, we construct hypoenergetic unicyclic and bicyclic graphs for above n.

Introduction

Let G be a simple graph with n vertices. Denote by Δ the maximum degree of a graph. The adjacency matrix $A(G)$ of G is a square matrix of order n, where (i, j)-entry is equal to 1 if the vertices v_i and v_j are adjacent, and is equal to 0 otherwise. The eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of G are said to be the eigenvalues of the graph and form

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it's spectrum. The nullity, denoted by n_0 (or $\eta(G)$), is the multiplicity of zero in the spectrum. The energy of G is defined as

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

McClelland (1971) gave the following general lower bound for the energy of a graph with n vertices and m edges:

$$\sqrt{2m + n(n-1)|detA|^{2/n}} .$$

Then $E(G) \geq n$ holds whenever all eigenvalues of the graph G differ from zero. In 2007, Nikiforov (see [2]) showed that for almost all graphs,

$$E = \left(\frac{4}{3\pi} + o(1)\right) n^{3/2} .$$

Thus the number of graphs satisfying the condition $E < n$ is relatively small. In [3], hypoenergetic graphs are defined to the graphs whose energy is less than the number of vertices. Recently, I. Gutman et al. (see [1]), have obtained results about hypoenergeitc trees. We now report that there exist hypoenergetic unicyclic graphs for all $n \geq 7$ and bicyclic graphs for $n \geq 8$.

Main results

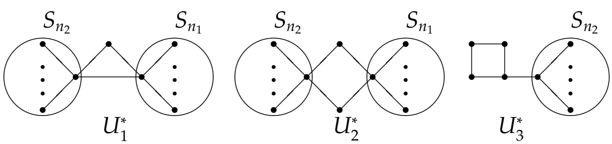
Denote by $\mathcal{U}$ the set of all n-vertex unicyclic graphs. Let U be a unicyclic graph of $\mathcal{U}$.

Lemma 1. [4] If the nullity of G is n_0 , then $E(G) \leq \sqrt{2m(n - n_0)}$.

Lemma 2. [5] Let $U \in \mathcal{U}$ ($n \geq 5$). Then $\eta(U) = n - 4$ if and only if

$$U \cong U_1^* \text{ or } U \cong U_2^* \text{ or } U \cong U_3^* .$$

$U_i^*(i = 1, 2, 3)$ is showed as the following graphs. In U_1^* and U_2^* , one of n_1 and n_2 might be equal 1, but the other must be equal or greater than 2.



Then by Lemma 2, the maximum nullity of an n-vertex unicyclic graph is $n-4$ $(n \geq 5)$.

Theorem 1. If $n \geq 7$, then there exist hypoenergetic unicyclic graphs for all n.

Proof. We consider two cases:

Case 1. $n = 7$ and $n = 8$.

U_4 is a unicyclic graph with $n = 7$ and U_5 with $n = 8$.

U_4 $\quad$ U_5

By direct calculation, $E(U_4) = 6.6468 < n = 7$ and $E(U_5) = 7.0733 < n = 8$.

Case 2. $n > 8$.

By Lemma 1, $E(U) \leq \sqrt{2n(n-n_0)}$. Now, if $\sqrt{2n(n-n_0)} < n$, then $n_0 > \frac{n}{2}$.

By Lemma 2, we arrive at the condition $n - 4 > \frac{n}{2}$, i. e., $n > 8$.

It follows from Case 1 and Case 2 that the Theorem holds. ∎

Theorem 2. If $n \leq 6$, then there exist no hypoenergetic unicyclic graphs.

Proof. By [7] (Table 1), it is easy to check that there exist no hypoenergetic unicyclic graphs for n =3, 4, 5. From [8] (Table 1), there are not hypoenergetic unicyclic graphs for $n = 6$. ∎

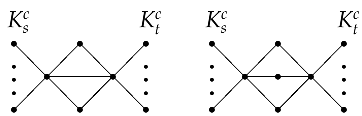
Let $\mathcal{B}$ be the set of all n-vertex bicyclic graphs and B be a bicyclic graph of $\mathcal{B}$.

Lemma 3. [6] Let $B \in \mathcal{B}$ and $\eta(B)$ be the nullity of B.

(1) $\eta(B) = n-2$ if and only if $B = K_{2,3}$; (2) $\eta(B) = n-3$ if and only if $B = K_4 - e$;

(3) $\eta(B) = n-4$ if and only if $B = B_i$ $(1 \leq i \leq 7)$.

Here we only depict B_6 and B_7:



$B_6(s,t) : 0 \leq s \leq t$ $\quad$ $B_7(s,t) : 0 \leq s \leq t$

Then by Lemma 3, the maximum nullity of an n-vertex bicyclic graph (except for $K_{2,3}$ and $K_4 - e$) is $n-4$.

Theorem 3. If $n = 5$ or $n \geq 8$, then there exist hypoenergetic bicyclic graphs for all n.

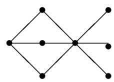
Proof. We consider three cases:

Case 1. $n = 5$.

By [7] (Table 1), there are five bicyclic graphs with $n = 5$ and $E(K_{2,3}) = 4.8990$. By computer calculation, $K_{2,3}$ is the only hypoenergetic bicyclic graph with $n = 5$.

Case 2. $n = 8$.

The following graph B_8 is a bicyclic graph with $n = 8$



B_8

By direct calculation, $E(B_8) = 7.7460 < 8$.

Case 3. $n \geq 9$.

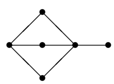
By Lemma 1, $E(B) \leq \sqrt{2(n+1)(n-n_0)}$. Now, if $\sqrt{2(n+1)(n-n_0)} < n$, then $n_0 > n - \frac{n^2}{2(n+1)}$. By Lemma 3, the maximum nullity n_0 is $n-4$. Thus $n - 4 > n - \frac{n^2}{2(n+1)}$. This inequality can be transformed into $n^2 - 8n - 8 > 0$, which are obeyed by all $n \geq 9$.

This completes the proof of Theorem 3. ∎

Theorem 4. If $n = 4, 6, 7$, then there exist no hypoenergetic bicyclic graphs.

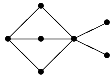
Proof. If $n = 4$, the only bicyclic graph is $K_4 - e$ and $E(K_4 - e) = 5.1231 > n = 4$.

By [7] (Table 1), there are 19 bicyclic graphs with $n = 6$. In these graphs, the minimal energy is $E = 6.4690 > n = 6$ and the graph is B_9.



B_9

By computer search and calculation, there are 68 bicyclic graphs with $n = 7$. The minimal energy of these graphs is $E = 7.1830 > n = 7$ and the graph is B_{10}.



B_{10}

∎

In the following, we consider the hypoenergetic unicyclic (bicyclic) graphs with n and Δ.

If G is either acyclic or contains exactly one cycle, according Sachs theorem and the Coulson integral formula, then [9,10]

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

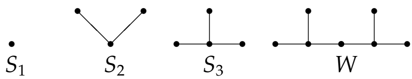
where $b_i(G) = |a_i(G)|$ and $a_i(G)$ is the i-th coefficient of characteristic polynomial of G. If $b_i(G_1) \geq b_i(G_2)$ for all $i \geq 0$ and there is a j such that $b_j(G_1) > b_j(G_2)$, then $E(G_1) > E(G_2)$.

Lemma 4. [11] Let G be a unicyclic graph . If G contains the cycle C_r ($r \not\equiv 0$ (mod 4)) and uv is an edge on this cycle, then $b_i(G) = b_i(G-uv) + b_{i-2}(G-u-v) + b_{i-r}(G-C_r)$.

Lemma 5. Let U be a unicyclic graph and e an edge contained in the cycle C_r ($r \not\equiv 0$ (mod 4)). Then $E(U-e) = E(T) < E(U)$.

Proof. By Lemma 4, $b_i(U) > b_i(U-uv)$. Then $E(U) > E(U-uv)$ ∎

Lemma 6. [1] There are no hypoenergetic trees with maximum degree at most 3, except S_1, S_2, S_3, W.



Theorem 5. Let U be a unicyclic graph with $\Delta \leq 3$. If U has a spanning tree $T \in \{S_2, S_3, W\}$, then U is not hypoenergetic.

Proof. Let T be a spanning tree of U. We consider three cases.

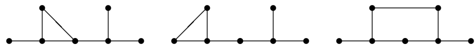
Case 1. $T \cong S_2$.

Then $U \cong C_3$ and $E(U) = E(C_3) = 4 > n = 3$.

Case 2. $T \cong S_3$.

Then U is the unicyclic graph with a triangle and a pendent vertex adjacent to one of vertices of the triangle. Then $E(U) = 4.9624 > n = 4$.

Case 3. $T \cong W$.



W_1 W_2 W_3

There are three unicyclic graphs with a spanning tree W. And $E(W_1) = 8.1709$, $E(W_2) = 8.2616$, $E(W_3) = 8.3184$, are greater than $n = 8$.

Thus the Theorem holds. ∎

Theorem 6. If U is a unicyclic graph with the cycle C_r ($r \not\equiv 0(mod 4)$) and maximum degree at most 3, then U is not a hypoenergetic unicyclic graph.

Proof. Let T be a spanning tree of U. If $T \in \{S_2, S_3, W\}$, by Theorem 5, then the result holds. Let U be a unicyclic graph with $T \notin \{S_2, S_3, W\}$ and e an edge of the cycle.

Suppose that U is hypoenergetic unicyclic graph. Then $E(U) < n$.

By Lemma 5, $E(T) = E(U - e) < E(U) < n$. Then $T = U - e$ is a hypoenergetic tree with maximum degree at most 3, by Lemma 6, a contradiction.

Hence the proof of Theorem 6 is completed. ∎

Theorem 7. If n is even and $\frac{n}{2} \le \Delta \le n-1$, then there exist hypoenergetic unicyclic graphs with Δ and n. If n is odd and $\frac{n+1}{2} \le \Delta \le n-1$, then there exist hypoenergetic unicyclic graphs with Δ and n.

Proof. Let n be even and $\Delta \in [\frac{n}{2}, n-2]$, $U = U_2^*$ with $S_{n_2} = S_{\Delta-1}$ and $S_{n_1} = S_{n-\Delta-1}$. By Lemma 2, $\eta(U) = n_0 = n - 4$.

Then $E(U) \le \sqrt{2n(n-n_0)} = \sqrt{2n \times 4} < n$ ($n > 8$).

If $\Delta = n-1$, let $U = U_1^*$ with $S_{n_1} = S_{n-2}$, then $\Delta(U) = n-1$ and $n_0 = n-4$. Hence

$E(U) < n$.

By the similar manner, the case that n is odd may be obtained. ∎

Theorem 8. Let B be a bicyclic graph. If n is even and $\Delta \in [\frac{n}{2}+1, n-1]$, then there exist hypoenergetic bicyclic graph with n and Δ. If n is odd and $\Delta \in [\frac{n+1}{2}, n-1]$, then there exist hypoenergetic graphs with n and Δ.

Proof. If n is even and $\Delta \in [\frac{n}{2}+1, n-2]$, let $B = B_7(\Delta-3, n-\Delta-2)$, by Lemma 3 (3), then $\eta(B) = n_0 = n-4$ and $E(B) \le \sqrt{2(n+1)(n-n_0)} = \sqrt{2(n+1)\times 4} < n$ $(n \ge 9)$.

If n is even and $\Delta = n-1$, let $B = B_6(0, \Delta-4)$, by Lemma 3 (3), then $n_0 = n-4$ and $E(B) \le \sqrt{2(n+1)(n-n_0)} = \sqrt{2(n+1)\times 4} < n$ $(n \ge 9)$.

The proof is fully analogous when n is odd. ∎

Acknowledgement: The authors would like to thank Professor I. Gutman for his valuable comments and suggestions, which have improved the presentation of the paper.

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