HYPOENERGETIC TREES

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(Received October 23, 2007)

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 $E(G) < n$. We formulate a sufficient (but not necessary) condition for an $n$-vertex tree with maximum vertex degree $\Delta$ being hypoenergetic. Based on it we show 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 $n \equiv k \pmod{4}$, $k = 0, 1, 3$; (c) if $\Delta \geq 5$, then there exist hypoenergetic trees for all $n \geq \Delta + 1$. We prove that hypoenergetic trees with $\Delta = 3$ exist only for $n = 4$ and $n = 7$ (a single such tree for each value of $n$). Computer search indicates that there exist hypoenergetic trees with $\Delta = 4$ also for $n \equiv 2 \pmod{4}$.
Introduction

Let $G$ be a graph on $n$ vertices, and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be its eigenvalues [1], that is, the eigenvalues of the adjacency matrix of $G$. The energy of $G$ is defined as

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

Although put forward already in the 1970s [2], and having much older roots in theoretical chemistry [3], the concept of graph energy has for a long time failed to attract the attention of mathematicians and mathematical chemists. However, around the year 2000, research on graph energy suddenly became a very popular topic, resulting in numerous significant discoveries, and in a remarkable number of publications.\(^1\)

For several classes of graphs it has been demonstrated that their energy exceeds the number of vertices. Among these are the regular graphs [11] and the hexagonal systems [15]. Based on a classical inequality of McClelland [18],

$$E(G) \geq \sqrt{2m + n(n-1)\det A}^{2/n}$$

where $m$ is the number of edges and $A$ the adjacency matrix, it is easy to verify that $E(G) \geq n$ holds whenever all eigenvalues of the graph $G$ differ from zero. Recently, Nikiforov [19] showed that for almost all graphs,

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

All these results suggest that graphs obeying the inequality $E < n$ should be relatively small in number, and that their characterization might be a feasible task. For obvious reasons these considerations should be restricted to connected graphs.

It was proposed [20] that the (connected) graphs whose energy is less than the number of vertices be referred to as “hypoenergetic”. Our first, computer-aided and chemistry-related studies of hypoenergetic graphs were communicated in the paper [20]. We now report some mathematical results on hypoenergetic trees, and show that with a few noteworthy exceptions, there exist hypoenergetic trees for any number of vertices and any value of the maximum vertex degree.

\(^1\)Since 2001 more than hundred papers on $E$ were produced, more than one per month. For some of the most recent works see [4–15], where references to earlier (yet also recent) articles can be found. For review of the theory of graph energy (as it was at the end of the last century) see [16]. For a recent review on the chemical aspects of $E$ see [17].
A sufficient condition

Let \( T \) denote a tree, let \( n \) be the number of its vertices, and let \( \Delta \) be the maximum degree of a vertex of \( T \). Then, of course, \( n \geq \Delta + 1 \). The nullity (= multiplicity of zero in the spectrum) of \( T \) will be denoted by \( n_0 \).

In what follows we assume that \( \Delta \geq 3 \). Namely, for \( \Delta \leq 2 \) the situation with regard to hypoenergeticity is simple: If \( \Delta = 0 \), then there exists a single one-vertex tree whose energy is equal to zero. This tree is, in a trivial manner, hypoenergetic. If \( \Delta = 1 \), then there exists a single two-vertex tree whose energy is equal to two. This tree is not hypoenergetic. For each value of \( n \), \( n \geq 3 \), there exists a unique \( n \)-vertex tree with \( \Delta = 2 \), the path \( P_n \), whose energy is well known [21]. Only \( P_3 \) is hypoenergetic.

For any graph \( G \) with \( n \) vertices and \( m \) edges, the McClelland upper bound for energy is [18] \( E(G) \leq \sqrt{2mn} \). If the nullity of \( G \) is \( n_0 \), then a simple improvement of this bound is [22] \( E(G) \leq \sqrt{2m(n-n_0)} \), which for trees becomes

\[
E(T) \leq \sqrt{2(n-1)(n-n_0)}. \tag{1}
\]

Equality in (1) is attained if and only if \( T \) is the \( n \)-vertex star. For \( n \geq 2 \) the \( n \)-vertex star is hypoenergetic. Therefore, in what follows, without loss of generality we may assume that \( T \) is not the star, in which case the inequality in (1) is strict. Now, if

\[
\sqrt{2(n-1)(n-n_0)} \leq n \tag{2}
\]

then the tree \( T \) will necessarily be hypoenergetic. Condition (2) can be rewritten as:

\[
n_0 \geq \frac{n(n-2)}{2(n-1)}. \tag{3}
\]

Fiorini et al. [23] proved that the maximum nullity of a tree with given values of \( n \) and \( \Delta \) is

\[
n - 2 \left\lfloor \frac{n-1}{\Delta} \right\rfloor \tag{4}
\]

and showed how trees with such nullity can be constructed.

Combining (3) and (4) we arrive at the condition

\[
n - 2 \left\lfloor \frac{n-1}{\Delta} \right\rfloor \geq \frac{n(n-2)}{2(n-1)} \tag{5}
\]
which, if satisfied, implies the existence of at least one hypoenergetic tree with \( n \) vertices and maximum vertex degree \( \Delta \).

**Solving the inequality (5)**

Finding the solutions of the inequality (5) is elementary, and we only sketch the reasoning that leads to the following:

**Lemma 1.** (a) If \( \Delta = 3 \), then the inequality (5) is satisfied only for \( n = 1, 2, 3, 4, 7 \).

(b) If \( \Delta = 4 \), then the inequality (5) is satisfied for all \( n \equiv 0 \ (mod \ 4) \), \( n \equiv 1 \ (mod \ 4) \), and \( n \equiv 3 \ (mod \ 4) \), as well as for \( n = 2 \).

(c) If \( \Delta \geq 5 \), then the inequality (5) is satisfied for all \( n \).

**Proof.** We first observe that

\[
\left[ \frac{n-1}{\Delta} \right] = \begin{cases} 
\frac{n}{\Delta} & \text{if } n \equiv 0 \ (mod \ \Delta) \\
\frac{(n-1)}{\Delta} & \text{if } 1 \equiv 0 \ (mod \ \Delta) \\
\frac{(n-k)}{\Delta} + 1 & \text{if } n \equiv k \ (mod \ \Delta), \ k = 2, 3, \ldots, \Delta - 1
\end{cases}
\]

by means of which the inequality (5) is transformed into

\[
n^2 - \frac{4n(n-1)}{\Delta} \geq 0 \quad \text{if } n \equiv 0 \ (mod \ \Delta) \quad (6)
\]

\[
n^2 - \frac{4(n-1)^2}{\Delta} \geq 0 \quad \text{if } n \equiv 1 \ (mod \ \Delta) \quad (7)
\]

\[
n^2 - 4(n-1) \left( \frac{n-k}{\Delta} + 1 \right) \geq 0 \quad \text{if } n \equiv k \ (mod \ \Delta), \ k = 2, 3, \ldots, \Delta - 1 \quad (8)
\]

Setting \( \Delta = 3 \) into the above relations, it is elementary to verify that (6) is satisfied only for \( n = 3 \), (7) only for \( n = 1, 4, 7 \), whereas (8) only for \( n = 2 \). This implies the claim (a) of the Lemma.

Assume now that \( \Delta \geq 4 \) and first consider the case \( n \equiv 2 \ (mod \ \Delta) \). Then inequality (8) is applicable (for \( k = 2 \)), and can be transformed into

\[
(n-2) [(\Delta - 4)(n-2) - 4] \geq 0 .
\]

This inequality is evidently satisfied for \( n = 2 \). If \( n > 2 \), then we arrive at

\[
(\Delta - 4)(n-2) - 4 \geq 0
\]
which does not hold for $\Delta = 4$, but holds for $\Delta > 4$.

If $n \equiv 0 \pmod{\Delta}$ and $n \equiv 1 \pmod{\Delta}$, then (6) and (7) are transformed into

$$n(\Delta - 4) + 4 \geq 0 \quad \text{and} \quad n^2(\Delta - 4) + 8n - 4 \geq 0$$

respectively, which are obeyed by all $n$. If $\Delta = 4$ and $n \equiv 3 \pmod{4}$, then (8) is reduced to $2n - 1 \geq 0$, which also holds for all respective values of $n$. By this we arrive at part (b) of Lemma 1.

It remains to verify that for $\Delta \geq 5$ and $3 \leq k \leq \Delta - 1$, the relation (8) is always satisfied. In order to do this, rewrite (8) as

$$(\Delta - 4)n^2 - 4(\Delta - k - 1)n + 4(\Delta - k) \geq 0$$

in which case the left-hand side is a quadratic polynomial in the variable $n$. Its value will be non-negative if the discriminant $D = [-4(\Delta - k - 1)]^2 - 16(\Delta - 4)(\Delta - k)$ is non-positive. Now, $D$ is a quadratic polynomial in the variable $k$. For both $k = 3$ and $k = \Delta - 1$, $D = -16(\Delta - 4)$, implying that the value of $D$ is negative for all $k$, $3 \leq k \leq \Delta - 1$.

By this the proof of Lemma 1 has been completed.

Bearing in mind that trees satisfying the condition (5) exist only if $n \geq \Delta + 1$, and that trees with nullity (4) always exist, we straightforwardly arrive at:

**Theorem 1.** 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 $n \equiv k \pmod{4}$, $k = 0, 1, 3$. (c) If $\Delta \geq 5$, then there exist hypoenergetic trees for all $n \geq \Delta + 1$.

In the subsequent section we prove that hypoenergetic trees with $\Delta = 3$ exist only for $n = 4$ and $n = 7$ (a single such tree for each value of $n$). Computer search indicates that there exist hypoenergetic trees with $\Delta = 4$ also for $n \equiv 2 \pmod{4}$. 
**Hypoenergetic trees with** $\Delta \leq 3$

Let $S_n$ denote the star on $n$ vertices and $W$ the 7-vertex tree, obtained from $P_3$ by adding a pendent vertex to the second vertex and to the fourth vertex, respectively. The tree $W$ is depicted in Fig. 1, where also the numbering of its vertices is indicated.

![Diagram of trees S1, S2, S3, and W](image)

**Fig. 1.** The hypoenergetic trees with maximum vertex degree not exceeding 3.

By computer search [20], one has shown that among trees with maximum degree at most 3 and order at most 22, $S_1, S_3, S_4$, and $W$ are the only hypoenergetic trees, see Fig. 1.

**Theorem 2.** There are no hypoenergetic trees with maximum degree at most 3, except $S_1, S_3, S_4$, and $W$.

**Proof.** As mentioned above, by checking all trees with $n$ vertices, $n \leq 22$, and maximum degree 3, it was found that $S_1, S_3, S_4$, and $W$ are the only hypoenergetic trees of order at most 22.

Our proof is based on the following observation. By deleting edges from a tree, the energy will strictly decrease. By deleting $k$ edges, $e_1, \ldots, e_k$, $k \geq 1$, from a tree $T$, it will decompose into $k + 1$ disconnected components $T_1, T_2, \ldots, T_{k+1}$, each component being a tree. If each of these components is not hypoenergetic, i.e., if $E(T_i) > n(T_i)$ for all $i = 1, 2, \ldots, k + 1$, then

$$E(T) > E(T - e_1 - \cdots - e_k) = E(T_1) + E(T_2) + \cdots + E(T_{k+1})$$

$$\geq n(T_1) + n(T_2) + \cdots + n(T_{k+1}) = n(T)$$

and, consequently, $T$ is also not hypoenergetic.
Now, we divide the trees with the maximum degree at most 3 into two classes:

**Class 1** contains the trees \( T \) that have an edge \( e \), such that \( T - e \cong T' \cup T'' \) and \( T', T'' \not\cong S_1, S_3, S_4, W \). **Class 2** contains the trees \( T \) in which there exists no edge \( e \), such that \( T - e \cong T' \cup T'' \) and \( T', T'' \not\cong S_1, S_3, S_4, W \), i.e., for any edge \( e \) of \( T \) at least one of \( T' \) or \( T'' \) is isomorphic to a tree in \( \{S_1, S_3, S_4, W\} \).

Then we distinguish between the following two cases:

**Case 1.** The tree \( T \) belongs to Class 1. Then we can use induction on the number \( n \) of vertices to verify that \( T \) is always hypoenergetic. For the first few values of \( n \) this is confirmed by direct calculation. Then by assuming that \( E(T') > n(T') \) and \( E(T'') > n(T'') \), from

\[
E(T) > E(T - e) = E(T') + E(T'') \geq n(T') + n(T'') = n(T)
\]

we conclude that also \( E(T) > n(T) \). This is the easy case.

**Case 2.** The tree \( T \) belongs to Class 2. Consider the center of \( T \). There are two subcases: either \( T \) has a (unique) center edge \( e \) or a (unique) center vertex \( v \).

**Subcase 2.1.** \( T \) has a center edge \( e \). The two fragments attached to \( e \) will be denoted by \( T' \) and \( T'' \). If so, then consider \( T - e \cong T' \cup T'' \).

**Subsubcase 2.1.1.** \( T' \) is isomorphic to a tree in \( \{S_1, S_3, S_4, W\} \), and if \( T' \cong W \), then it is attached to the center edge \( e \) through the vertex 3, but not through a pendent vertex (these are vertices 1, 5, 6, 7, see Fig. 1). Then it is easy to see that the order of \( T \) is at most 14. Hence, if \( T \) is not isomorphic to an element of \( \{S_1, S_3, S_4, W\} \), then \( T \) is not hypoenergetic.

**Subsubcase 2.1.2.** \( W \) is attached to the center edge \( e \) through a pendent vertex. Then we need to distinguish between the situations shown in Fig. 2.

If the other end vertex of the center edge \( e \) is of degree 2 (see diagram A in Fig. 2), then \( T'' \) has at least 5 and at most 16 vertices. Consequently, \( T \) has at least 12 and at most 23 vertices. If the number of vertices is between 12 and 22 we known that \( T \) is not hypoenergetic. If \( n = 23 \), then by deleting the edge \( f \) from \( T \) we get a 6-vertex and a 17-vertex fragment, neither of which being hypoenergetic. Then \( T \) is not hypoenergetic because of (9).
Fig. 2. Explanation of the notation used in the proof of Theorem 2.

If the other end vertex of the center edge $e$ is of degree 3, then the structure of the tree $T$ is as shown in diagram B in Fig. 2. Each fragment $T_a, T_b$ must have at least 4 and at most 15 vertices. If neither $T_a \cong W$ nor $T_b \cong W$, then the subgraph $T - f - g$ consists of three components, each with not more than 15 vertices, none of which being hypoenergetic. Then $E(T - f - g) > n$ and we are done. If $T_a \cong W$, but $T_b \not\cong W$, then we have to delete the edges $g$ and $h$ resulting, again, in three non-hypoenergetic fragments. Finally, if both $T_a, T_b \cong W$, then $T$ has 21 vertices and is thus not hypoenergetic.

**Subcase 2.2.** $T$ has a center vertex $v$. If $v$ is of degree two, then the two fragments attached to it will be denoted by $T'$ and $T''$. If $v$ is of degree three, then the three fragments attached to it will be denoted by $T'$, $T''$, and $T'''$.

**Subsubcase 2.2.1.** $T'$ is isomorphic to a tree in $\{S_1, S_3, S_4, W\}$, and if $T' \cong W$, then it is attached to the center edge $e$ through the vertex 3, but not through a pendent vertex. Then it is easy to see that the order of $T$ is at most 22. Hence, if $T$ is not isomorphic to an element of $\{S_1, S_3, S_4, W\}$, then $T$ is not hypoenergetic.

**Subsubcase 2.2.2.** $W$ is attached to the center vertex $v$ through a pendent vertex. Then we need again to distinguish between the situations shown in Fig. 2.
If the degree of $v$ is two (see diagram C is Fig. 2), then the fragment $T''$ has at least 5 and at most 15 vertices. Therefore $T$ has at least 12 and at most 23 vertices. If $T$ has less than 23 vertices, we are done. If $n(T) = 23$, then by deleting the edge $f$ we obtain fragments that are 8- and a 15-vertex trees, thus not hypoenergetic, and (9) is applicable.

If the center vertex $v$ is of degree three (see diagram D in Fig. 2), then both fragments $T''$ and $T'''$ have at least 5 and at most 15 vertices. If $T'', T''' \not\cong W$, then $T - f - g$ consists of three fragments, none of which being hypoenergetic and (9) is applicable. If $T'' \cong W$, but $T''' \not\cong W$, then instead of $T - f - g$ one needs to consider $T - g - h$ and to proceed analogously. If both $T'' \cong W$, and $T''' \cong W$, then $T$ has 22 vertices and is thus again not hypoenergetic.

By this all possible cases have been exhausted, and the proof of Theorem 2 is completed.

Discussion

Relation (5) is a sufficient, but not a necessary condition for the existence of hypoenergetic trees. Therefore, if for some $n$ and $\Delta$ the inequality (5) does not hold, it still may happen that there exist $n$-vertex hypoenergetic trees with maximum vertex degree $\Delta$.

Indeed, the computer search reported in [20] showed that there exist hypoenergetic trees with $\Delta = 4$ and $n = 6, 10, 14, 18, 22$, namely for the first five even integers greater than 2, not divisible by 4. In view of this, we formulate the following:

Conjecture. There exist $n$-vertex hypoenergetic trees with $\Delta = 4$ for any $n \equiv 2 \ (mod \ 4) \ , \ n > 2$. Consequently, there exist $n$-vertex hypoenergetic trees with $\Delta = 4$ for any $n \ , \ n \geq 5$.

In the computer search reported in [20], the $n$-vertex trees with $\Delta = 3$ and with minimum energy were found, up to $n = 22$. No generally valid regularity in their structure could be observed. We mention in passing that Lin et al. [24] characterized the $n$-vertex trees with maximum degree $\Delta$ and minimum energy, but only for $\Delta \geq$
\[(n + 1)/3\]. For smaller values of \(\Delta\), in particular for \(\Delta = 3\) and \(\Delta = 4\) [25], the structure of the minimum-energy trees remains an unsolved (probably difficult) problem.

**Acknowledgement:** I.G. thanks the colleagues from the Center for Combinatorics of the Nankai University, for making him possible to stay at this institution in the Fall of 2007. X.L., Y.S. and J.Z. would like to acknowledge the support of PCSIRT, NSFC and the “973” program.

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