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HYPOENERGETIC TREES

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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 Δ 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 $n \equiv k \ (mod\ 4)$, $k = 0, 1, 3$; (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 $n \equiv 2 \ (mod\ 4)$.

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],

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

where m is the number of edges and $\mathbf{A}$ 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 Δ 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 Δ is

$$n - 2\left\lceil \frac{n-1}{\Delta} \right\rceil \tag{4}$$

and showed how trees with such nullity can be constructed.

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

$$n - 2\left\lceil \frac{n-1}{\Delta} \right\rceil \geq \frac{n(n-2)}{2(n-1)} \tag{5}$$

which, if satisfied, implies the existence of at least one hypoenergetic tree with n vertices and maximum vertex degree Δ.

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

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

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

$$n^2 - \frac{4n(n-1)}{\Delta} \geq 0 \qquad \text{if } \ n \equiv 0 \ (mod\ \Delta) \tag{6}$$

$$n^2 - \frac{4(n-1)^2}{\Delta} \geq 0 \qquad \text{if } \ n \equiv 1 \ (mod\ \Delta) \tag{7}$$

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

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

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

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 $n \equiv 0 \ (mod\ \Delta)$ and $n \equiv 1 \ (mod\ \Delta)$, then (6) and (7) are transformed into

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

respectively, which are obeyed by all n. If $\Delta = 4$ and $n \equiv 3 \ (mod\ 4)$, 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 $n \equiv k \ (mod\ 4)$, $k = 0, 1, 3$. (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 $n \equiv 2 \ (mod\ 4)$.

Hypoenergetic trees with $\Delta \leq 3$

Let S_n denote the star on n vertices and W the 7-vertex tree, obtained from P_5 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.

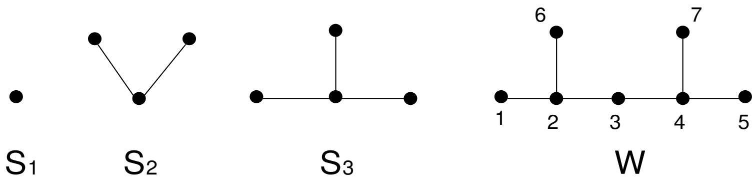

Fig. 1. The hypoenergetic trees with maximum vertex degree not exceeding 3.

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

$$\begin{aligned} E(T) &> E(T - e_1 - \cdots - e_k) = E(T_1) + E(T_2) + \cdots + E(T_{k+1}) \\ &\geq n(T_1) + n(T_2) + \cdots + n(T_{k+1}) = n(T) \end{aligned} \tag{9}$$

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 $T', T'' \ncong S_1, S_3, S_4, W$. **Class 2** contains the trees T in which there exists no edge e, such that $T - e \cong T' \cup T''$ and $T', T'' \ncong S_1, S_3, S_4, W$, 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).

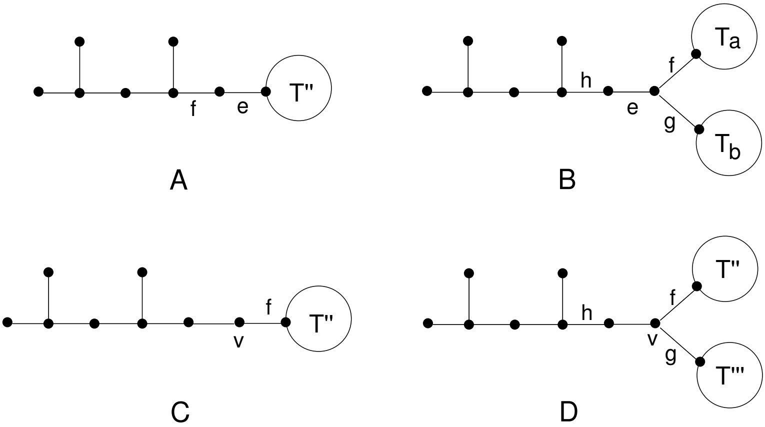

Fig. 2. Explanation of the notation used in the proof of Theorem 2.

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 $T_b \ncong W$, 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 $T'', T''' \ncong W$, then $T - f - g$ consists of three fragments, none of which being hypoenergetic and (9) is applicable. If $T'' \cong W$, but $T''' \ncong W$, 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 Δ the inequality (5) does not hold, it still may happen that there exist n-vertex hypoenergetic trees with maximum vertex degree Δ.

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 Δ and minimum energy, but only for $\Delta \geq$

$\lceil (n+1)/3 \rceil$. For smaller values of Δ, in particular for $\Delta = 3$ and $\Delta = 4$ [25], the structure of the minimum–energy trees remains an unsolved (probably difficult) problem.

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