Note for Nikiforov’s two conjectures on the energy of trees

Xueliang Li, Jianxi Liu
Center for Combinatorics and LPMC-TJKLC
Nankai University, Tianjin 300071, P.R. China
Email: lxl@nankai.edu.cn

Abstract

The energy $E$ of a graph is defined to be the sum of the absolute values of its eigenvalues. Nikiforov in “V. Nikiforov, The energy of $C_4$-free graphs of bounded degree, Lin. Algebra Appl. 428(2008), 2569–2573” proposed two conjectures concerning the energy of trees with maximum degree $\Delta \leq 3$. In this short note, we show that both conjectures are true.

Key words: energy of a graph, conjecture, tree

AMS Subject Classification: 05C50, 05C90, 15A18, 92E10

Let $G$ be a graph on $n$ vertices and $\lambda_1, \lambda_2, \cdots, \lambda_n$ be the eigenvalues of its adjacency matrix. The value $E(G) = |\lambda_1| + \cdots + |\lambda_n|$ is defined as the energy of $G$, which has been studied intensively, see [1, 3] for a survey.

In [5], Nikiforov proposed two conjectures on the energy of trees. In order to state and prove them, we need the following notations and terminology.

The complete $d$-ary tree of height $h-1$ is denoted by $C_h$, which is built up inductively as follows: $C_1$ is a single vertex and $C_h$ has $d$ branches $C_{h-1}, \cdots, C_{h-1}$. See Figure 1 for examples. It is convenient to set $C_0$ as the empty graph.

Let $T_{n,d}$ be the set of all trees with $n$ vertices and maximum degree $d+1$. We define a special tree $T_{n,d}^*$ as follows (see also [4]):

Definition 1 $T_{n,d}^*$ is the tree with $n$ vertices that can be decomposed as in Figure 2.
with \( B_{k,1}, \ldots, B_{k,d-1} \in \{ C_k, C_{k+2} \} \) for \( 0 \leq k < l \) and either \( B_{l,1} = \cdots = B_{l,d} = C_{l-1} \) or \( B_{l,1} = \cdots = B_{l,d} = C_l \) or \( B_{l,1}, \ldots, B_{l,d} \in \{ C_l, C_{l+1}, C_{l+2} \} \), where at least two of \( B_{l,1}, \ldots, B_{l,d} \) equal \( C_{l+1} \). This representation is unique, and one has the “digital expansion”

\[
(d - 1)n + 1 = \sum_{k=0}^{l} a_k d^k,
\]

where \( a_k = (d - 1)(1 + (d + 1)r_k) \) and \( 0 \leq r_k \leq d - 1 \) is the number of \( B_{k,i} \) that are isomorphic to \( C_{k+2} \) for \( k < l \), and

- \( a_l = 1 \) if \( B_{l,1} = \cdots = B_{l,d} = C_{l-1} \),
- \( a_l = d \) if \( B_{l,1} = \cdots = B_{l,d} = C_l \),
- or otherwise \( a_l = d + (d - 1)q_l + (d^2 - 1)r_l \), where \( q_l \geq 2 \) is the number of \( B_{l,i} \) that are isomorphic to \( C_{l+1} \) and \( r_l \) is the number of \( B_{l,i} \) that are isomorphic to \( C_{l+2} \).

Let \( B_n \) denote the tree constructed by taking three disjoint copies of the complete 2-ary tree of height \( h - 1 \), i.e., \( C_n \), and joining an additional vertex to their roots (i.e., vertices of height zero). In the end of [5], Nikiforov formulated two conjectures as follows:

**Conjecture 2** The limit

\[
c = \lim_{n \to \infty} \frac{E(B_n)}{3 \cdot 2^{n+1} - 2}
\]

exists and \( c > 1 \).

**Conjecture 3** Let \( \epsilon > 0 \). If \( T \) is a sufficiently large tree with \( \Delta(T) \leq 3 \), then \( E(T) \geq (c - \epsilon)|T| \).

*Supported by NSFC No.10831001, PCSIRT and the “973” program.*
Nikiforov mentioned that empirical data given in [2] seem to corroborate these conjectures, but apparently new techniques are necessary to prove or disprove them. We will give confirmative proofs for both Conjecture 2 and Conjecture 3.

We first state two known lemmas from [4], which will be needed in the sequel.

**Lemma 4** [4]. Let \( n \) and \( d \) be positive integers. Then \( T_{n,d}^* \) is the unique (up to isomorphism) tree in \( T_{n,d} \) that minimizes the energy.

**Lemma 5** [4]. The energy of \( T_{n,d}^* \) is asymptotically

\[
E(T_{n,d}^*) = \alpha_d \cdot n + O(\ln n),
\]

where

\[
\alpha_d = 2\sqrt{d(d-1)^2} \left( \sum_{j \equiv 0 \pmod{2}} d^{-j} \left( \cot \frac{\pi}{2j} - 1 \right) + \sum_{j \equiv 1 \pmod{2}} d^{-j} \left( \csc \frac{\pi}{2j} - 1 \right) \right)
\]

(2)

is a constant that only depends on \( d \).

| \( d \) | \( \alpha_d \) |
|---|---|
| 2 | 1.102947505597 |
| 3 | 0.970541979946 |
| 4 | 0.874794345784 |
| 5 | 0.802215758706 |
| 6 | 0.744941364903 |
| 7 | 0.698315075830 |
| 8 | 0.659425329682 |
| 9 | 0.626356806404 |
| 10 | 0.607794680849 |
| 20 | 0.43453264777 |
| 50 | 0.279574397741 |
| 100 | 0.198836515295 |

Table 1 Some numerical values for the constant \( \alpha_d \).

With the above two lemmas, the two conjectures can be proved very easily as follows.

**Theorem 6** The limit

\[
c = \lim_{n \to \infty} \frac{E(B_n)}{3 \cdot 2^{n+1} - 2}
\]

exists and \( c > 1 \).
Proof. We just need to notice that $B_n$ is exactly the tree $T_{3,2^n+1}^*$ with $l = n$, $B_{k,1} = C_k$ for $0 \leq k < l$, $B_{1,1} = B_{1,2} = C_n$. Therefore, by Lemma 5 and Table 1 we have

\[
\lim_{n \to \infty} \left( \frac{E(B_n)}{3 \cdot 2^{n+1} - 2} \right) = \lim_{n \to \infty} \left( \alpha_2 + \frac{O(\ln(3 \cdot 2^{n+1} - 2))}{3 \cdot 2^{n+1} - 2} \right) = \alpha_2 > 1.
\]

In fact, from Lemmas 4 and 5 we have that for any $T \in T_{n,d}$,

\[
E(T) \geq E(T_{n,d}^*) = \alpha_d \cdot n + O(\ln n).
\]

Therefore, we obtain

**Theorem 7** Let $\epsilon > 0$. If $T$ is a sufficiently large tree with $\Delta(T) = d + 1$, then $E(T) \geq (\alpha_d - \epsilon)|T|$, where $\alpha_d$ is given in Equ. (2).

Letting $d = 2$, we get

**Corollary 8** Let $\epsilon > 0$. If $T$ is a sufficiently large tree with $\Delta(T) = 3$, then $E(T) \geq (\alpha_2 - \epsilon)|T|$, where $\alpha_2$ is given in Equ. (2).

Recall that a hypoenergetic graph of order $n$ is such that $E(G) < n$, whereas it is strongly hypoenergetic if $E(G) < n - 1$. We have the following easy remarks:

**Remark 1**: From Lemma 5 and Table 1, one can see that there is neither strongly hypoenergetic tree nor hypoenergetic tree of order $n$ and maximum degree $\Delta$ for $\Delta \leq 3$ and any suitable large $n$.

**Remark 2**: From Lemma 5 and Table 1, one can also see that there are both hypoenergetic trees and strongly hypoenergetic trees of order $n$ and maximum degree $\Delta$ for $\Delta \geq 4$ and any suitable large $n$.

**References**

[1] I. Gutman, Topology and stability of conjugated hydrocarbons: The dependence of total $\pi$-electron energy on molecular topology, *J. Serb. Chem. Soc.* 70 (2005), 441–456.

[2] I. Gutman, On graphs whose energy exceeds the number of vertices, *Lin. Algebra Appl.* 429(11-12) (2008), 2670–2677.

[3] I. Gutman, X. Li, J. Zhang, Graph Energy, in: M. Dehmer, F. Emmert-Streib (Eds.), Analysis of Complex Networks: From Biology to Linguistics, Wiley-VCH Verlag, Weinheim, 2009, pp.145-174.
[4] C. Heuberger, S. Wagner, Chemical tress minimizing energy and Hosoya index, *J. Math. Chem.* 46(1) (2009), 214–230.

[5] V. Nikiforov, The energy of $C_4$-free graphs of bounded degree, *Lin. Algebra Appl.* 428 (2008), 2569–2573.