MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **59** (2008) 315-320

ISSN 0340 - 6253

EXTREMAL ENERGY TREES

Ivan Gutman,[a] Slavko Radenković,[a]
Nana Li[b] and Shuchao Li[b]

[a] *Faculty of Science, University of Kragujevac,*
P. O. Box 60, 34000 Kragujevac, Serbia
e-mail: gutman@kg.ac.yu ; slavko.radenkovic@gmail.com

[b] *Faculty of Mathematics and Statistics, Central China Normal University,*
Wuhan 430079, P. R. China
e-mail: linanama@hotmail.com ; lscmath@mail.ccnu.edu.cn

(Received July 11, 2007)

Abstract

The results of the preceding paper [N. Li, S. Li, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 000–000] are completed by determining the n-vertex trees with second–, third–, fourth–, fifth–, sixth–, and seventh–minimal energy, as well as those with second–, third–, and fourth–maximal energy, for all values of n.

INTRODUCTION

If G is a graph on n vertices, and $\lambda_1, \lambda_2, \ldots, \lambda_n$ are its eigenvalues, then the *energy* of G is defined as [1, 2]

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

In a paper published long time ago [3] the n-vertex trees with maximal and second–maximal energy were determined, as well as the n-vertex trees with minimal, second–minimal, third–minimal, and fourth–minimal energy. In a recent work [4] these results were extended by determining the n-vertex trees with third–maximal, fifth–minimal, sixth–minimal, and seventh–minimal energy. However, all these results were stated under the assumption that n is sufficiently large, whereas the extremal–energy trees with smaller number of vertices have not been characterized. The aim of the present note is to fill this gap.

The results reported in this paper are obtained by combining the (mathematically proven) claims from [3, 4] with a systematic computer–aided search, performed on all n-vertex trees with small values of n.

SOME EXTREMAL TREES

The n-vertex path P_n is the n-vertex tree in which no vertex has degree greater than two. The vertices of P_n are labelled consecutively by $1, 2, \ldots, n$. It is known [3] that P_n has the greatest energy among n-vertex trees, and that this holds for all $n \geq 1$.

The n-vertex star S_n is the n-vertex tree in which one vertex has degree $n-1$ and (therefore) all other vertices are pendent. The vertex of degree $n-1$ is said to be the center of S_n. It is known [3] that S_n has the smallest energy among n-vertex trees, and that this holds for all $n \geq 1$.

Adopting the notation from the paper [4] we define the following trees:

- For $n \geq 3$, the tree Y_n is obtained by attaching a pendent vertex to a pendent vertex of S_{n-1}.
- For $n \geq 5$, the tree Z_n is obtained by connecting the central vertices of S_{n-3} and S_3.

- For $n \geq 5$, the tree W_n is obtained by connecting the central vertex of S_{n-3} with vertex 1 of P_3.
- For $n \geq 6$, the tree D_n is obtained by connecting the central vertices of S_{n-4} and S_4.
- For $n \geq 6$, the tree U_n is obtained by connecting the central vertex of S_{n-4} with a pendent vertex of S_4.
- For $n \geq 7$, the tree Q_n is obtained by connecting the central vertices of S_{n-5} and S_5.
- For $n \geq 6$, the tree Q'_n is obtained by connecting the central vertex of S_{n-4} with vertex 2 of P_4.
- For $n \geq 5$, the tree $P_{n-2}(3)2$ is obtained by connecting vertex 3 of P_{n-2} with vertex 1 of P_2.
- For $n \geq 7$, the tree $P_{n-2}(5)2$ is obtained by connecting vertex 5 of P_{n-2} with vertex 1 of P_2.
- For $n \geq 9$, the tree $P_{n-2}(7)2$ is obtained by connecting vertex 7 of P_{n-2} with vertex 1 of P_2.

MINIMAL–ENERGY TREES

In [3, 4] the first few trees with minimal energy were determined. We are now able to slightly sharpen these results. For the sake of brevity, instead of "*tree with k-th minimal energy*" we will say "*k-th minimal tree*". Further, all trees considered below are assumed to have n vertices.

Theorem 1. For $n \leq 3$ there is no second–minimal tree. For $n \geq 4$ the second–minimal tree is Y_n.

Theorem 2. For $n \leq 4$ there is no third–minimal tree. For $n = 5$ the third–minimal tree is T_1 depicted in Fig. 1 (which is just the 5-vertex path). For $n \geq 6$ the third–minimal tree is Z_n.

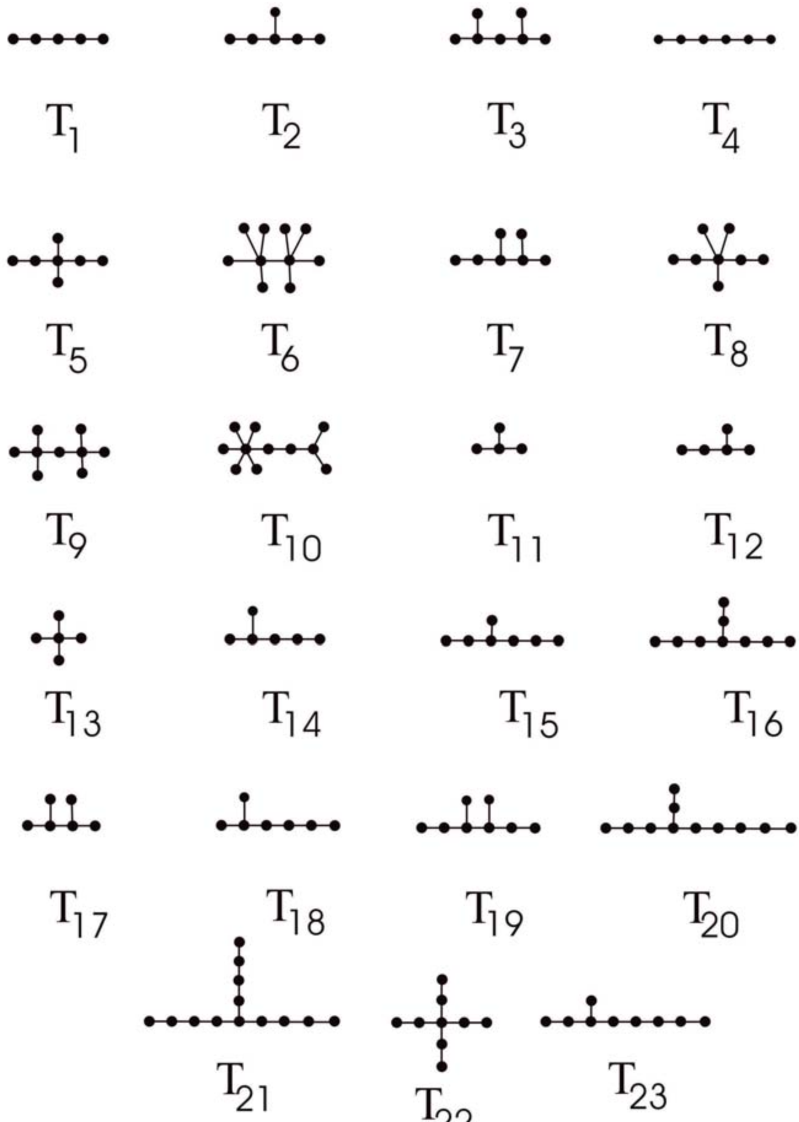
T_1
T_2
T_3
T_4
T_5
T_6
T_7
T_8
T_9
T_{10}
T_{11}
T_{12}
T_{13}
T_{14}
T_{15}
T_{16}
T_{17}
T_{18}
T_{19}
T_{20}
T_{21}
T_{22}
T_{23}

Figure 1

Theorem 3. For $n \leq 5$ there is no fourth–minimal tree. For $n \geq 6$ the fourth–minimal tree is W_n. Exceptionally, for $n = 8$ the trees W_n and D_n are cospectral, and therefore W_8 and D_8 share the fourth– and fifth–minimal position.

Theorem 4. For $n \leq 5$ there is no fifth–minimal tree. For $n = 6$ and $n = 7$ the fifth–minimal trees are T_2 and T_3, respectively, depicted in Fig. 1. As mentioned in Theorem 3, for $n = 8$ the cospectral trees W_8 and D_8 are fourth/fifth–minimal. For $n \geq 9$ the fifth–minimal tree is D_n.

Theorem 4 provides a slight correction of the claim in [4] that D_n is fifth–minimal already for $n \geq 6$.

Theorem 5. For $n \leq 5$ there is no sixth–minimal tree. For $n = 6$, $n = 7$, and $n = 10$ the sixth–minimal trees are T_4, T_5, and T_6, respectively, depicted in Fig. 1. For $n = 11$ the trees U_n and Q_n are cospectral, and therefore U_{11} and Q_{11} share the sixth– and seventh–minimal position. For $n = 8$, $n = 9$, and $n \geq 12$ the sixth–minimal tree is U_n.

In the preceding work [4] it was established that (for sufficiently large n) the seventh–minimal tree is either Q_n or Q'_n. Our numerical calculations clearly indicate that Q'_n is not seventh–minimal for any value of n. More specifically, we obtained the following:

Theorem 6. For $n \leq 6$ there is no seventh–minimal tree. For $n = 7$, $n = 8$, $n = 9$, and $n = 10$ the seventh–minimal trees are T_7, T_8, T_9, and T_{10}, respectively, depicted in Fig. 1. As mentioned in Theorem 5, for $n = 11$ the cospectral trees W_{11} and Q_{11} are sixth/seventh–minimal. For $n \geq 12$ the seventh–minimal tree is Q_n.

MAXIMAL–ENERGY TREES

In this section, for the sake of brevity, instead of "*tree with k-th maximal energy*" we will say "*k-th maximal tree*". Again, all trees considered are assumed to have n vertices.

In [3] the maximal and second–maximal trees were determined, and in [4] also the third–maximal. We are now going to slightly sharpen these results and, in addition, to conjecture which the fourth–maximal tree could be.

Theorem 7. For $n \leq 3$ there is no second–maximal tree. For $n = 4$ and $n = 5$ the second–maximal trees are T_{11} and T_{12}, respectively, depicted in Fig. 1. For $n \geq 6$ the second–maximal tree is $P_{n-2}(3)2$.

Theorem 8. For $n \leq 4$ there is no third–maximal tree. For $n = 5$, $n = 6$, $n = 7$, and $n = 9$ the third–maximal trees are T_{13}, T_{14}, T_{15}, and T_{16}, respectively, depicted in Fig. 1. For $n = 8$ and $n \geq 10$ the third–maximal tree is $P_{n-2}(5)2$.

Conjecture 9. For $n \leq 5$ there is no fourth–maximal tree. For $n = 6$, $n = 7$, $n = 8$, $n = 11$, and $n = 13$ the fourth–maximal trees are T_{17}, T_{18}, T_{19}, T_{20}, and T_{21}, respectively, depicted in Fig. 1. For $n = 9$ there are two cospectral trees, T_{22} and T_{23} sharing the fourth– and fifth–maximal position. For $n = 10$, $n = 12$, and $n \geq 14$ the fourth–maximal tree is $P_{n-2}(7)2$.

References

[1] I. Gutman, The energy of a graph, *Ber. Math.–Statist. Sekt. Forschungsz. Graz* **103** (1978) 1–22.

[2] I. Gutman, The energy of a graph: Old and new results, in: A. Betten, A. Kohnert, R. Laue, A. Wassermann (Eds.), *Algebraic Combinatorics and Applications*, Springer–Verlag, Berlin, 2001, pp. 196–211.

[3] I. Gutman, Acyclic systems with extremal Hückel π-electron energy, *Theor. Chim. Acta* **45** (1977) 79–87.

[4] N. Li, S. Li, On the extremal energy of trees, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 291–314.