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EQUIENERGETIC AND ALMOST–EQUIENERGETIC TREES

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Abstract

The energy $E(G)$ of a graph G is equal to the sum of the absolute values of the eigenvalues of G. Two graphs G_a and G_b are said to be equienergetic if $E(G_a) = E(G_b)$. Numerous families of non-cospectral equienergetic graphs have been reported so far. However, until now it was not noticed that there exist pairs of graphs whose energies differ insignificantly. We refer to such graphs as almost–equienergetic. A detailed study of almost–equienergetic trees is provided.

INTRODUCTION

Let G be a graph on n vertices and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be its eigenvalues (or more precisely: the eigenvalues of the adjacency matrix of G) [1, 2]. Then the *energy* of G is defined as

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

For details on graph energy and its chemical applications see the books [2, 3], the reviews [4–6], and the references cited therein.

The concept of *equienergetic graphs* was introduced in 2004, independently by Balakrishnan [7] and Brankov et al. [8]. Two graphs G_a and G_b are said to be equienergetic if $E(G_a) = E(G_b)$. For obvious reasons one is interested only in non-cospectral equienergetic graphs.

Equienergetic graphs attracted recently much attention [9–23] and several constructions of such graphs have been put forward. Equienergetic trees were considered already in the paper [8], but until now no general method for their construction is known. The only procedure by which pairs (or greater families) of non-cospectral equienergetic trees could be detected is computer–aided search, using the computed values of the energy. When a pair of non-cospectral trees is found to have energies equal within the accuracy of the applied numerical procedure, then these trees need to be further examined in order to prove the true equality of their energies.

We illustrate this on the triplet of trees T_1, T_2, T_3, depicted in Fig. 1, whose energies (calculated up to four decimal places) were found to be equal to $E = 21.4205$.

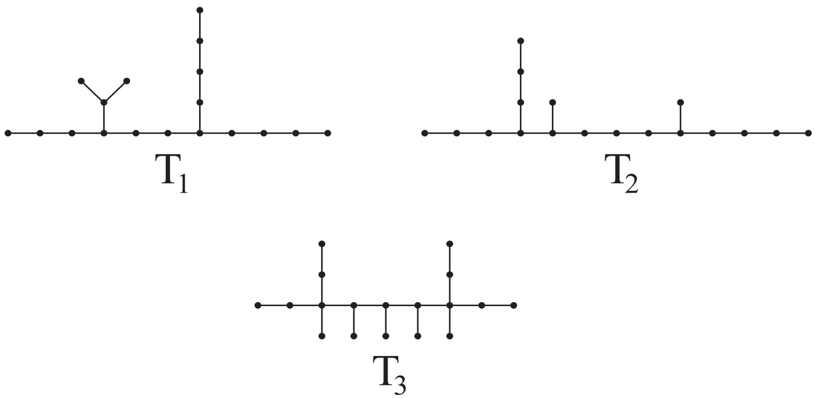

Fig. 1. Three trees whose equienergeticity can be exactly proven.

Using standard recursive techniques [1, 3], we can compute the characteristic polynomials of these trees:

$$\begin{aligned}\phi(T_1,\lambda) &= \lambda^{18} - 17\,\lambda^{16} + 117\,\lambda^{14} - 421\,\lambda^{12} + 853\,\lambda^{10} - 973\,\lambda^{8} + 588\,\lambda^{6}\\ &- 164\,\lambda^{4} + 16\,\lambda^{2}\end{aligned}$$

$$\begin{aligned}\phi(T_2,\lambda) &= \lambda^{18} - 17\,\lambda^{16} + 117\,\lambda^{14} - 421\,\lambda^{12} + 853\,\lambda^{10} - 973\,\lambda^{8} + 588\,\lambda^{6}\\ &- 164\,\lambda^{4} + 16\,\lambda^{2}\end{aligned}$$

$$\begin{aligned}\phi(T_3,\lambda) &= \lambda^{18} - 17\,\lambda^{16} + 111\,\lambda^{14} - 359\,\lambda^{12} + 632\,\lambda^{10} - 632\,\lambda^{8} + 359\,\lambda^{6} \\ &- 111\,\lambda^{4} + 17\,\lambda^{2} - 1\ .\end{aligned}$$

Because the coefficients of the characteristic polynomial are integers, the above expressions are exact. We immediately see that $\phi(T_1,\lambda) \equiv \phi(T_2,\lambda)$, implying that T_1 and T_2 are cospectral and therefore, in a trivial manner, equienergetic. On the other hand, $\phi(T_3,\lambda)$ differs from the characteristic polynomials of T_1 and T_2. Consequently, T_1 and T_3 are not cospectral.

By elementary algebraic reasoning it can be shown that the polynomials $\phi(T_1,\lambda)$ and $\phi(T_3,\lambda)$ can be factorized as:

$$\begin{aligned}\phi(T_1,\lambda) &= \lambda^2\,(\lambda^2-1)(\lambda^2-2)^2\,(\lambda^2-4)(\lambda^4-3\,\lambda^2+1)(\lambda^4-5\,\lambda^2+1) \\ \phi(T_3,\lambda) &= (\lambda^2-1)^3\,(\lambda^4-3\,\lambda^2+1)(\lambda^4-5\,\lambda^2+1)(\lambda^4-6\,\lambda^2+1)\end{aligned}$$

from which the spectra of these two trees are readily computed:

$$Sp(T_1) = \left\{0\,,\,0\,,\,\pm 1\,,\,\pm\sqrt{2}\,,\,\pm\sqrt{2}\,,\,\pm 2\,,\,\pm\sqrt{\frac{3\pm\sqrt{5}}{2}}\,,\,\pm\sqrt{\frac{5\pm\sqrt{21}}{2}}\right\}$$

$$Sp(T_3) = \left\{\pm 1\,,\,\pm 1\,,\,\pm 1\,,\,\pm\sqrt{\frac{3\pm\sqrt{5}}{2}}\,,\,\pm\sqrt{\frac{5\pm\sqrt{21}}{2}}\,,\,\pm\sqrt{\frac{6\pm\sqrt{32}}{2}}\right\}\ .$$

The respective energies are then:

$$E(T_1) = 6 + 4\sqrt{2} + 2\left(\sqrt{\frac{3+\sqrt{5}}{2}} + \sqrt{\frac{3-\sqrt{5}}{2}} + \sqrt{\frac{5+\sqrt{21}}{2}} + \sqrt{\frac{5-\sqrt{21}}{2}}\right)$$

$$\begin{aligned}E(T_3) &= 6 + 2\left(\sqrt{\frac{3+\sqrt{5}}{2}} + \sqrt{\frac{3-\sqrt{5}}{2}} + \sqrt{\frac{5+\sqrt{21}}{2}} + \sqrt{\frac{5-\sqrt{21}}{2}}\right. \\ &+ \left.\sqrt{\frac{6+\sqrt{32}}{2}} + \sqrt{\frac{6-\sqrt{32}}{2}}\right)\ .\end{aligned}$$

In order to verify that the right–hand sides of the above two expressions are equal, we recall the identity

$$\sqrt{\frac{x+\sqrt{x^2-4}}{2}} + \sqrt{\frac{x-\sqrt{x^2-4}}{2}} = \sqrt{x+2}$$

the application of which readily renders

$$E(T_1) = E(T_3) = 6 + 4\sqrt{2} + 2\sqrt{5} + 2\sqrt{7}\ .$$

Thus we have completed the proof that T_1, T_2, T_3 form a family of equienergetic trees of the type $2+1$ (cf. Table 1).

There exist pairs of trees for which the above described procedure is not easy to be accomplished, but which nevertheless seem to be exactly equienergetic. Such are, for instance, the trees T_4 and T_5, depicted in Fig. 2.

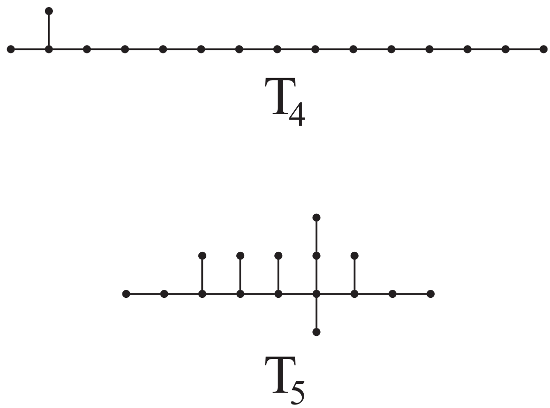

Fig. 2. Two trees believed to be exactly equienergetic, but whose equienergeticity is difficult to be be exactly proven.

The energies of T_4 and T_5 agree up to the first 50 decimal places (as computed by *Mathematica*):

$$\begin{aligned} E(T_4) &= 19.02872890844516985936794290989136493329753629030132\cdots \\ E(T_5) &= 19.02872890844516985936794290989136493329753629030132\cdots\ . \end{aligned}$$

Their characteristic polynomials may be factorized as:

$$\begin{aligned} \phi(T_4,\lambda) &= \lambda^2\,(\lambda^2-3)(\lambda^4-5\,\lambda^2+5)(\lambda^8-7\,\lambda^6+14\,\lambda^4-8\,\lambda^2+1) \\ \phi(T_5,\lambda) &= (\lambda^8-8\,\lambda^6+14\,\lambda^4-7\,\lambda^2+1)(\lambda^8-7\,\lambda^6+14\,\lambda^4-8\,\lambda^2+1) \end{aligned}$$

which makes the proof of the validity of the equality $E(T_4) = E(T_5)$ very difficult (yet not impossible).

The smallest two non-cospectral equienergetic trees have $n = 9$ vertices and were first reported in [8]. In [8] is shown that for $n = 9$ this pair is unique.

ALMOST–EQUIENERGETIC TREES

Intending to accomplish a detailed and complete search for families of equienergetic non-cospectral n-vertex trees, for n as large as technically possible, we encountered unexpected computational difficulties. After much stray we realized that in addition to strictly equienergetic non-cospectral trees, there also exist trees whose energies are different, but remarkably close. These we refer to as *almost–equienergetic* trees.

A pair of almost–equienergetic trees, T_6, T_7, that appears to be smallest, is depicted in Fig. 3. Their energies (calculated by means of *Mathematics*) are

$$E(T_6) = 18.090756640280765\cdots$$
$$E(T_7) = 18.090756641775140\cdots$$

which means that $|E(T_6) - E(T_7)| \approx 1.5 \cdot 10^{-9}$.

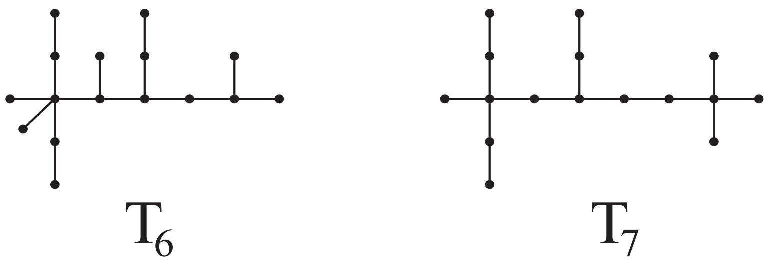

Fig. 3. A pair of almost–equienergetic trees on 16 vertices. Provided the criterion for almost–equienergeticity is given by Eq. (1), this seems to be the smallest pair of almost–equienergetic trees.

What "remarkably close" means for the energy of two graphs is a theme for debate. Based on our numerical experience, we tentatively and to a great degree arbitrarily call two graphs G_a and G_b *almost–equienergetic* if

$$0 < |E(G_a) - E(G_b)| < 10^{-8} . \tag{1}$$

By accepting this convention we examined all n-vertex trees with $9 \leq n \leq 22$, searching for families whose energies differ by less than 10^{-8}. By this we embraced both the class of equienergetic and almost–equienergetic trees. Except in a few cases, no attempt was made to recognize which of these families pertain to equienergetic and which to almost–equienergetic species. The main results obtained are presented in Table 1. Additional results can be obtained from the authors, upon request.

One of the greatest families detected, is depicted in Fig. 4. It consists of 7 trees $T_8, T_9, \ldots, T_{14}$ (all with $n = 22$). The trees T_8 and T_9 are cospectral, T_{10}, T_{11}, T_{12}, and T_{13} are cospectral (but not cospectral with T_8, T_9), whereas T_{14} has spectrum different from all other members of this family. The respective energies are

$$\begin{aligned} E(T_8) &= 24.41317462670817367737401699982 9\cdots \\ E(T_{10}) &= 24.413174625652754496385602383841\cdots \\ E(T_{14}) &= 24.413174628345991390665163085679\cdots \end{aligned}$$

ALMOST–LAPLACIAN–EQUIENERGETIC TREES

The *Laplacian energy* of a graph G is defined as [24, 25]

$$LE(G) = \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right|$$

where n is the number of vertices, m the number of edges, and μ_i , $i = 1, 2, \ldots, n$, are the Laplacian eigenvalues (or more precisely: the eigenvalues of the Laplacian matrix of G). In full analogy with energy, if the conditions

$$LE(G_a) = LE(G_b) \qquad \text{and} \qquad 0 < |LE(G_a) - LE(G_b)| < 10^{-8}$$

are satisfied, we speak of Laplacian– equienergetic and Laplacian–almost–equienergetic graphs, respectively.

n	$\#fam$	$size$	$type$
9	1	2	$1+1$
10	0		
11	0		
12	0		
13	1	2	$1+1$
14	1	2	$1+1$
15	4	2	$1+1$
16	8	2	$1+1$
	1	3	$2+1$
17	3	2	$1+1$
	1	3	$2+1$
18	20	2	$1+1$
	4	3	$2+1$
19	86	2	$1+1$
	25	3	$2+1$
	7	4	$3+1$
	2	4	$2+2$
	1	5	$2+3$
	1	6	$3+3$
	1	7	$2+5$
20	487	2	$1+1$
	136	3	$2+1$
	8	4	$3+1$
	10	4	$2+2$
	3	5	$3+2$
	1	5	$4+1$
	1	6	$5+1$
	1	8	$5+3$
21	3176	2	$1+1$
	678	3	$2+1$
	4	3	$1+1+1$
	95	4	$3+1$
	47	4	$2+2$
	2	4	$2+1+1$

n	$\#fam$	$size$	$type$
21	16	5	$3+2$
	24	5	$4+1$
	1	5	$3+1+1$
	8	6	$5+1$
	1	6	$3+3$
	1	6	$4+2$
	1	7	$6+1$
	1	7	$4+3$
	2	7	$5+2$
	1	8	$6+2$
	1	9	$5+4$
22	22929	2	$1+1$
	3952	3	$2+1$
	101	3	$1+1+1$
	566	4	$3+1$
	193	4	$2+2$
	28	4	$2+1+1$
	109	5	$4+1$
	54	5	$3+2$
	6	5	$2+2+1$
	1	5	$3+1+1$
	30	6	$5+1$
	3	6	$3+2+1$
	10	6	$4+2$
	6	6	$3+3$
	1	6	$4+1+1$
	5	7	$6+1$
	2	7	$4+3$
	1	7	$5+2$
	1	7	$4+2+1$
	1	8	$7+1$
	1	8	$5+3$
	1	9	$6+3$

Table 1. Families of n-vertex trees whose energies differ by less than 10^{-8}. For $n \leq 8$ there are no such families. $\#fam$ is the number of families of a given size and a given type. Type $x+y$ indicates that x members of the family are mutually cospectral, and y other members are also mutually cospectral, but not cospectral with the former group; the meaning of type $x+y+z$ is analogous.

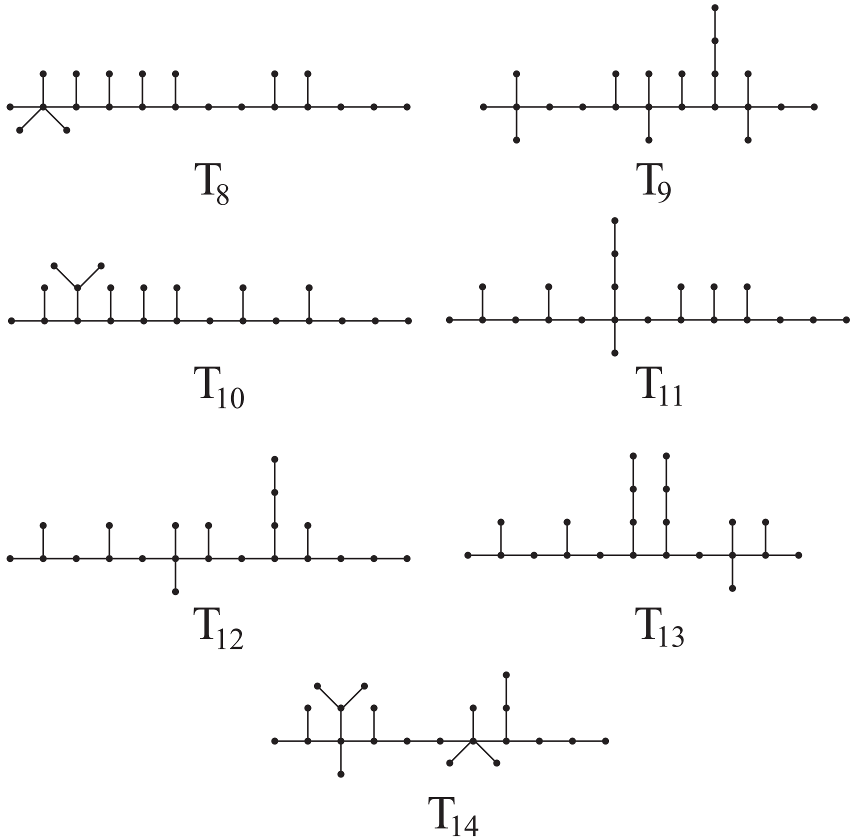

Fig. 4. A seven–membered family of (type 4 + 2 + 1) of almost–equienergetic 22-vertex trees (cf. Table 1).

The results of our computer–based search for trees of this kind are presented in Table 2. We mention here that we were not able to identify a single pair of Laplacian–equienergetic trees (which, however, does not mean that such trees do not exist). More details on this matter can be found in the subsequent paper [26].

n	$\#fam$	size	type
16	1	2	1+1
17	1	2	1+1
18	22	2	1+1
19	119	2	1+1
20	694	2	1+1
	42	3	2+1
	1	4	2+2
21	4905	2	1+1
	6	3	1+1+1
	3	3	2+1
22	32674	2	1+1
	6	3	2+1
	147	3	1+1+1

Table 2. Families of n-vertex trees whose Laplacian energies differ by less than 10^{-8}. For $n \leq 15$ there are no such families. Other details are same as in Table 1.

References

[1] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs — Theory and Application*, Academic Press, New York, 1980.

[2] D. Cvetković, M. Doob, I. Gutman, A. Torgašev, *Recent Results in the Theory of Graph Spectra*, Elsevier, Amsterdam, 1988.

[3] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer–Verlag, Berlin, 1986.

[4] 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.

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

[6] 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, Weinheim, in press.

[7] R. Balakrishnan, The energy of a graph, *Lin. Algebra Appl.* **387** (2004) 287–295.

[8] V. Brankov, D. Stevanović, I. Gutman, Equienergetic chemical trees, *J. Serb. Chem. Soc.* **69** (2004) 549–553.

[9] H. S. Ramane, H. B. Walikar, S. B. Rao, B. D. Acharya, P. R. Hampiholi, S. R. Jog, I. Gutman, Equienergetic graphs, *Kragujevac J. Math.* **26** (2004) 5–13.

[10] H. S. Ramane, I. Gutman, H. B. Walikar, S. B. Halkarni, Another class of equienergetic graphs, *Kragujevac J. Math.* **26** (2004) 15–18.

[11] H. S. Ramane, H. B. Walikar, S. B. Rao, B. D. Acharya, P. R. Hampiholi, S. R. Jog, I. Gutman, Spectra and energies of iterated line graphs of regular graphs, *Appl. Math. Lett.* **18** (2005) 679–682.

[12] H. S. Ramane, I. Gutman, H. B. Walikar, S. B. Halkarni, Equienergetic complement graphs, *Kragujevac J. Sci.* **27** (2005) 67–74.

[13] G. Indulal, A. Vijayakumar, On a pair of equienergetic graphs, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 83–90.

[14] H. S. Ramane, H. B. Walikar, Construction of equienergetic graphs, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 203–210.

[15] L. Xu, Y. Hou, Equienergetic bipartite graphs, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 363–370.

[16] G. Indulal, A. Vijayakumar, Classes of Türker equivalent graphs, *Graph Theory Notes New York* **53** (2007) 30–36.

[17] W. López, J. Rada, Equienergetic digraphs, *Int. J. Pure Appl. Math.* **36** (2007) 361–372.

[18] G. Indulal, A. Vijayakumar, A note on energy of some graphs, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 269–274.

[19] J. Liu, B. Liu, Note on a pair of equienergetic graphs, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 275–278.

[20] A. S. Bonifácio, C. T. M. Vinagre, N. M. M. de Abreu, Constructing pairs of equienergetic and non-cospectral graphs, *Appl. Math. Lett.* **21** (2008) 338–341.

[21] H. S. Ramane, I. Gutman, D. S. Revankar, Distance equienergetic graphs, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 473–484.

[22] G. Indulal, A. Vijayakumar, Equienergetic self–complementary graphs, *Czech. Math. J.*, in press.

[23] C. K. Li, W. So, Construction of graphs with equienergetic subgraphs, *Lin. Multilin. Algebra*, in press.

[24] I. Gutman, B. Zhou, Laplacian energy of a graph, *Lin. Algebra Appl.* **414** (2006) 29–37.

[25] B. Zhou, I. Gutman, On Laplacian energy of graphs, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 211–220.

[26] J. Liu, B. Liu, S. Radenković, I. Gutman, Minimal LEL-equienergetic graphs, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 000–000 (subsequent paper).