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MINIMAL LEL–EQUIENERGETIC GRAPHS

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Abstract

Let G be a graph with n vertices and m edges. Let $\mu_1, \mu_2, \ldots, \mu_n$ be the Laplacian eigenvalues of G. The Laplacian–energy–like graph invariant $LEL(G) = \sum_{i=1}^{n} \sqrt{\mu_i}$, has been recently defined and investigated by two of present authors [J. Liu, B. Liu, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 355–372.]. Two non-isomorphic graphs G_1 and G_2 of the same order are said to be LEL-equienergetic if $LEL(G_1) = LEL(G_2)$. In this paper we consider LEL-equienergetic and almost–LEL-equienergetic graphs and find that they occur relatively rarely. If the criterion for almost–LEL-equienergeticity is $|LEL(G_1) - LEL(G_2)| < 10^{-8}$, then for $n \leq 14$ there are no pairs of non-cospectral LEL-equienergetic or almost–LEL-equienergetic trees, but there exist two almost–equienergetic pairs for $n = 15$.

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1 INTRODUCTION

Let G be a simple undirected graph on n vertices and m edges. Let $\mathbf{A}$ be the symmetric $(0,1)-$adjacency matrix of G and $\mathbf{D} = diag(d_1, d_2, \ldots, d_n)$ be the diagonal matrix of vertex degrees. The Laplacian matrix of G is $\mathbf{L} = \mathbf{D} - \mathbf{A}$. Let λ_1, λ_2,..., λ_n be the adjacency spectrum of G, and let μ_1, μ_2,..., μ_n be the Laplacian spectrum of G.

The energy $E(G)$ of a graph G is defined as $E(G) = \sum\limits_{i=1}^{n} |\lambda_i|$ [7]. This quantity has a clear connection to chemical problems [8–10] and has recently been much investigated (see [11, 12, 14, 15, 26, 28] and the references cited therein). Two non-isomorphic graphs G_1 and G_2 of the same order are said to be equienergetic [2] if $E(G_1) = E(G_2)$. Certainly, cospectral graphs are equienergetic. Such a case is of no interest for us, and in what follows we are concerned with pairs of non-cospectral graphs.

We may think of $E(G)$ as a mapping $E : \mathbf{G} \mapsto \mathbf{R}$, where $\mathbf{G}$ is the set of all graphs, $\mathbf{R}$ is the field of real numbers. Obviously, E is not a monomorphism. In fact, there exist pairs of equienergetic non-cospectral connected graphs of order n for $n = 6$ and $n \geq 8$ [17]. For other results on equienergetic graphs see [1,2,16,17,19–25].

In a recent study [19] it was found that in addition to pairs of equienergetic graphs (for which $E(G_1) - E(G_2) = 0$), there exist pairs of so-called *almost–equienergetic graphs*, for which the difference $E(G_1) - E(G_2)$ is non-zero, but (from a practical point of view) negligibly small. In the present work, we consider two graphs G_1 and G_2 to be almost–equienergetic if the difference $|E(G_1) - E(G_2)|$ is non-zero, but smaller than 10^{-k}, where, tentatively, $k = 8$.

In the same sense, we have pairs of almost-LE-equienergetic and almost-LEL-equienergetic graphs.

The Laplacian energy $LE(G)$ of a graph G has been defined [13] as $LE(G) = \sum\limits_{i=1}^{n} \left|\mu_i - \frac{2m}{n}\right|$. For recent investigations of this quantity see [27]. Similarly as in the case of graph energy, two non-isomorphic graphs G_1 and G_2 of the same order are said to be LE-equienergetic if $LE(G_1) = LE(G_2)$. In this paper, we show that there exists a pair of LE-equienergetic non-cospectral connected graphs of order n for all $n \geq 4$.

The Laplacian-energy-like invariant of a graph G, defined as $LEL(G) = \sum\limits_{i=1}^{n} \sqrt{\mu_i}$, has recently been defined and investigated [18]. Similarly, two non-isomorphic graphs G_1 and G_2 of the same order are said to be LEL-equienergetic if $LEL(G_1) = LEL(G_2)$.

The quantities $E(G)$, $LE(G)$ and $LEL(G)$ were found to have a number of analogous properties [13, 18]. Since the ordinary energy E has a long known application in molecular orbital theory of organic molecules (see [8–10]), we preconceive that LE and LEL would also have some chemical applications; for the first results along these lines see [3]. Note that from the point of view of (chemical) applications it is immaterial whether two graphs are equienergetic or almost–equienergetic.

In the following we discuss LEL-equienergetic graphs and find that they occur relatively rarely. We present three pairs of connected, non-cospectral LEL-equienergetic graphs. Finally, we report the results of a computer–aided search for non-cospectral LEL-equienergetic trees.

2 MAIN RESULTS

Theorem 2.1. *There exist pairs of connected, non-cospectral LE-equienergetic graphs of order n, for all $n \geq 4$.*

Proof. Let $G = K_n$ be the complete graph on n vertices, and let $H = K_{1,n-1}+\{e\}$ be the graph obtained from the star graph with n vertices by adding to it an edge. Then by direct computing we have that $LE(G) = LE(H) = 2(n-1)$, for all $n \geq 4$. □

However, for all connected graphs up to 7 vertices (for the graphs, see [4–6]), by direct computing we found that there are no connected, non-cospectral LEL-equienergetic graphs. So the pairs of LEL-equienergetic graphs are not so numerous. Oppositely, there are many pairs of LE-equienergetic graphs of order $n \leq 7$. Hence, the minimal examples of connected, non-cospectral LEL-equienergetic graphs are the graphs of order 8.

We now present three pairs of connected, non-cospectral LEL-equienergetic graphs.

Example 2.1. *Let G_{801} and G_{802} be the graphs shown in Fig. 1. Their Laplacian spectra are $\{6,6,4,4,4,2,2,0\}$ and $\{8,6,6,4,4,1,1,0\}$, respectively. It is then immediate to verify that $LEL(G_{801}) = LEL(G_{802})$.*

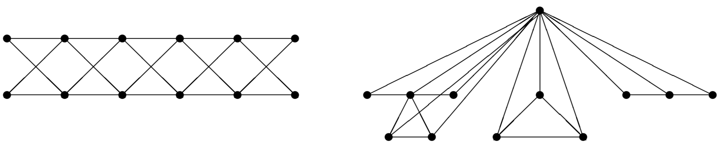
G_{801} **Fig. 1.** G_{802}

Example 2.2. *Let* G_{803} *and* G_{804} *be the graphs shown in Fig 2. Since their Laplacian spectra are* $\{6,4,4,4,2,2,2,0\}$ *and* $\{8,6,4,4,2,1,1,0\}$ *, respectively, it is straightforward to check that* $LEL(G_{803}) = LEL(G_{804})$ *.*

G_{803} **Fig. 2.** G_{804}

Note that all the Laplacian eigenvalues in the Examples 2.1 and 2.2 are integers. The following example gives a graph whose Laplacian matrix has irrational eigenvalues.

Example 2.3. *Let* G_{1201} *and* G_{1202} *be the graphs shown in Fig. 3. Since the Laplacian spectrum of* G_{1201} *is* $\{4+2\sqrt{3},6,4,4,4,4,4,2,2,2,4-2\sqrt{3},0\}$ *whereas the Laplacian spectrum of* G_{1202} *is* $\{12,6,4,4,4,4,2,2,2,1,1,0\}$ *, we have that* $LEL(G_{1201}) = LEL(G_{1202})$ *.*



G_{1201} **Fig. 3.** G_{1202}

In what follows we assume that the exponent k is equal to 8. By direct computing, we found that up to 15 vertices, there are no non-cospectral LE-equienergetic or almost–LE-equienergetic trees (i. e., for all such trees the difference between the LE-values is greater than 10^{-8}). Further, up to 14 vertices, there are no non-cospectral LEL-equienergetic or almost-LEL-equienergetic trees. For $n = 16$ there exists a single pair of almost–LE-equienergetic trees, depicted in Fig. 4. For $n = 15$ there exist two pairs of almost–LEL-equienergetic trees, also depicted in Fig. 4.

The respective LE– and LEL-values are the following:

$$LE(T_1) = 23.3873831394 \qquad LE(T_2) = 23.3873831433$$

$$LEL(T_3) = 17.9122842889 \qquad LEL(T_4) = 17.9122842846$$

$$LEL(T_5) = 17.6944539702 \qquad LEL(T_4) = 17.6944539712$$

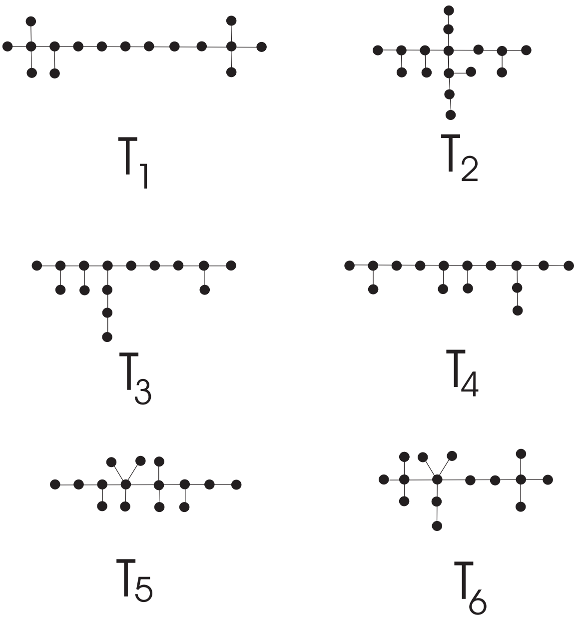


Fig. 4. If the criterion for almost–LE-equienergeticity and almost–LEL-equienergeticity of two trees T_a and T_b is $|LE(T_a) - LE(T_b)| < 10^{-k}$; $k = 8$ and $|LEL(T_a) - LEL(T_b)| < 10^{-k}$; $k = 8$, respectively, then the trees T_1 and T_2 are the smallest two non-Laplacian-cospectral almost–LE-equienergetic species ($n = 16$). There are two pairs (T_3, T_4) and (T_5, T_6) of non-Laplacian-cospectral almost–LEL-equienergetic trees with the smallest number ($n = 15$) of vertices. Pairs of non-Laplacian-cospectral LE-equienergetic trees as well as of non-Laplacian-cospectral LEL-equienergetic trees were not detected.

That the differences between the above LE– and LEL-values are not a result of rounding errors in our FORTRAN program was checked by using a MATHEMATICA software that (exactly) computes LE and LEL on 100 decimals.

Within our search, we did not recognize any pair of LE-equienergetic or LEL-equienergetic trees, so that finding of such pairs remains a task for the future.

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