EQUIENERGETIC GRAPHS

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Abstract. The energy of a graph is the sum of the absolute values of its eigenvalues. Two graphs are said to be equienergetic if their energies are equal. We show how infinitely many pairs of equienergetic graphs can be constructed, such that these graphs are connected, possess equal number of vertices, equal number of edges, and are not cospectral.

INTRODUCTION

The concept of graph energy was introduced by one of the present authors long time ago [9]. Recently this concept started to attract considerable attention of mathematicians involved in the study of graph spectral theory; for recent mathematical works on the energy of graphs see [1,3,7,8,10–12,15–23,25–33]. The chemical aspects of this concept are outlined in due detail in the book [13].

Let G be a graph on n vertices. The eigenvalues of the adjacency matrix of G, denoted by $\lambda_1, \lambda_2, \dots, \lambda_n$, are said to be the eigenvalues of G, and form the spectrum of G [5].

The energy of the graph G is then defined as

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

If for two graphs, G_1 and G_2 , the equality $E(G_1) = E(G_2)$ is satisfied, then G_1 and G_2 are said to be *equienergetic*. For obvious reasons, cospectral graphs are equienergetic. The less trivial case are pairs of equienergetic, non-cospectral graphs.

Examples of equienergetic, non-cospectral graphs are easily found. Because the union of a graph and an arbitrary number of isolated vertices has the same energy as the graph itself, we are not interested in "examples" of this kind. The simplest non-trivial example is formed by the triangle and the quadrangle (G_a and G_b in Fig. 1); their eigenvalues are 2, -1, -1 and 2, 0, 0, -2, respectively and therefore $E(G_a) = E(G_b) = 4$. The simplest equienergetic graphs with non-integer energies are the 4-vertex path (G_c in Fig. 1) and the 6-vertex star (G_d), with eigenvalues $\sqrt{(3+\sqrt{5})/2}$, $\sqrt{(3-\sqrt{5})/2}$, $-\sqrt{(3-\sqrt{5})/2}$, $-\sqrt{(3+\sqrt{5})/2}$ and $\sqrt{5}, 0, 0, 0, -\sqrt{5}$, respectively, both having energy equal to $2\sqrt{5}$. In addition to the quadrangle G_b , there are two more non-cospectral 4-vertex graphs, having energy equal to 4: G_e (with eigenvalues 1, 1, -1, -1) and G_f (with eigenvalues 2, 0, -1, -1). These graphs are not connected. The smallest pair of non-cospectral, connected equienergetic graphs with the same number of vertices are the pentagon (G_g) and the tetragonal pyramid (G_h), whose eigenvalues are 2, $(\sqrt{5}-1)/2$, $(\sqrt{5}-1)/2$, $-(\sqrt{5}+1)/2$, $-(\sqrt{5}+1)/2$ and $\sqrt{5}+1,0,0,-\sqrt{5}+1,-2$, respectively, and for which $E(G_g)=E(G_h)=2\sqrt{5}+2$.

If we restrict ourselves to connected graphs, and if we require that both equienergetic mates have the same number of vertices, then examples of the above type,

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possessing larger number of vertices, are much more difficult to find. Anyway, in the existing literature, no systematic way seems to have been ever reported for constructing pairs of connected, equienergetic, non-cospectral graphs with equal number of vertices. In what follows we provide such a construction.

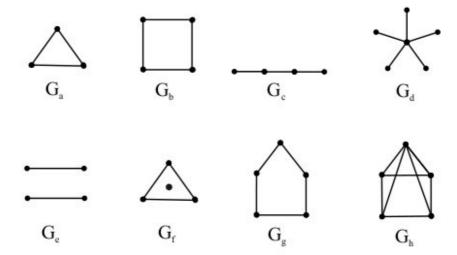


Fig. 1. Non-cospectral equienergetic graphs with small number of vertices: $E(G_a) = E(G_b) = E(G_e) = E(G_f) = 4$, $E(G_c) = E(G_d) = 2\sqrt{5}$, $E(G_g) = E(G_h) = 2\sqrt{5} + 2$.

ON LINE GRAPHS OF REGULAR GRAPHS

Let G be a graph, and $L^1(G)=L(G)$ its line graph [14]. Let, further, $L^2(G)=L(L^1(G))$, $L^3(G)=L(L^2(G))$, ..., $L^k(G)=L(L^{k-1}(G))$, ..., be the iterated line graphs of G.

A graph is said to be regular of degree r if all its vertices have degrees equal to r. As it is well known [14], the line graph of a regular graph is also regular. More precisely, if G is a regular graph on n vertices, of degree r, then L(G) is a regular graph on

$$n_1 = \frac{1}{2} n r \tag{1}$$

vertices, of degree

$$r_1 = 2r - 2. (2)$$

Consequently, all iterated line graphs $L^k(G)$ of a regular graph G are regular graphs. In particular, if G is a regular graph on n vertices, of degree r, $r \geq 2$, then by a repeated application of Eqs. (1) and (2) we see that $L^2(G)$ is a regular graph on

$$n_2 = \frac{1}{2} n_1 r_1 = \frac{1}{2} \left(\frac{1}{2} n r \right) (2r - 2) = \frac{1}{2} n r (r - 1)$$

vertices, of degree

$$r_2 = 2r_1 - 2 = 2(2r - 2) - 2 = 4r - 6$$
.

THE MAIN RESULT

Theorem 1. Let G_1 and G_2 be two regular graphs, both on n vertices, both of degree $r \geq 3$. Then $L^2(G_1)$ and $L^2(G_2)$ are equienergetic.

Proof. We show that the energy of the second iterated line graph of a regular graph of degree $r \geq 3$ depends only on the number of vertices and on the degree r.

Let G be a regular graph on n vertices, of degree $r \geq 3$. Let its eigenvalues be λ_i , i = 1, 2, ..., n. Then, according to a long–known result by Sachs [24] (Theorem 2.15 in [5]), the eigenvalues of L(G) are:

$$\lambda_i + r - 2 \qquad i = 1, 2, \dots, n, \text{ and}
-2 \qquad n(r-2)/2 \text{ times}$$
(3)

Bearing in mind the (above specified) structure of $L^2(G)$, and by a two-fold application of Eq. (3), we conclude that the eigenvalues of $L^2(G)$ are:

$$\lambda_i + 3r - 6$$
 $i = 1, 2, ..., n$, and $2r - 6$ $n(r - 2)/2$ times, and -2 $n \cdot r(r - 2)/2$ times . (4)

If d_{max} is the greatest vertex degree of a graph, then all its eigenvalues belong to the interval $[-d_{max}, +d_{max}]$ [5]. In particular, the eigenvalues of a regular graph of degree r satisfy the condition $-r \le \lambda_i \le +r$ for all $i=1,2,\ldots,n$. If $r\geq 3$, then $3\,r-6\geq 3$, and because of $\lambda_i\geq -r$, we have $\lambda_i+3\,r-6\geq 0$. If $r\geq 3$, then $2\,r-6\geq 0$.

We thus see that all negative–valued eigenvalues of $L^2(G)$ are equal to -2, and that they occur in the spectrum of $L^2(G)$ nr(r-2)/2 times.

Bearing this in mind, the energy of $L^2(G)$ is computed from (4) as follows:

$$E(L^{2}(G)) = \sum_{i=1}^{n} (\lambda_{i} + 3r - 6) + \frac{1}{2}n(r - 2) \times (2r - 6) + \frac{1}{2}nr(r - 2) \times |-2|$$

which, by taking into account that the sum of the eigenvalues of G is zero [5], readily yields:

$$E(L^2(G)) = 2 n r(r-2)$$
. (5)

From Eq. (5) we see that the second iterated line graphs of all regular graphs, having the same number of vertices and having the same degree, are mutually equienergetic. This is tantamount to the statement of Theorem 1.

Corollary 1.1. Let G_1 and G_2 be two regular graphs, both on n vertices, both of degree $r \geq 3$. Then for any $k \geq 2$, $L^k(G_1)$ and $L^k(G_2)$ are equienergetic.

Proof. The statement of Corollary 1.1 for k=2 coincides with Theorem 1. Therefore we assume that $k \geq 3$.

The fact that $L^{k-2}(G_1)$ and $L^{k-2}(G_2)$ have equal number of vertices follows from a repeated application of Eqs. (1) and (2). Because $L^{k-2}(G_1)$ and $L^{k-2}(G_2)$ are regular graphs of the same degree, possessing equal number of vertices, by Theorem 1, $L^k(G_1) = L^2(L^{k-2}(G_1))$ and $L^k(G_2) = L^2(L^{k-2}(G_2))$ are equienergetic.

Corollary 1.2. Let G_1 and G_2 be two connected and non-cospectral regular graphs, both on n vertices, both of degree $r \geq 3$. Then for any $k \geq 2$, both $L^k(G_1)$ and $L^k(G_2)$ are regular, connected, non-cospectral and equienergetic. Furthermore, $L^k(G_1)$ and $L^k(G_2)$ possess the same number of vertices, and the same number of edges.

Proof. The line graph of a graph without isolated vertices is connected if and

only if the graph itself is connected [14]. Hence, if G is connected, then $L^k(G)$ is also connected, $k \geq 1$. According to (3), if G_1 and G_2 are not cospectral, then also $L^1(G_1)$ and $L^1(G_2)$ are not cospectral. Thus, $L^k(G_1)$ and $L^k(G_2)$ are not cospectral for any $k \geq 1$.

From the proof of Corollary 1.1 we know that $L^k(G_1)$ and $L^k(G_2)$ possess equal number of vertices. From the fact that the number of edges of $L^k(G)$ is equal to the number of vertices of $L^{k+1}(G)$ follows that $L^k(G_1)$ and $L^k(G_2)$ have also equal number of edges. \Box

DISCUSSION

Theorem 1 and, in particular, its Corollary 1.2 provide a general method for constructing families of mutually non-cospectral equienergetic graphs, each member of which is connected and has the same number of vertices. One simply has to find a pertinent collection of mutually non-cospectral connected regular graphs (of degree greater than two) and to construct their k-th iterated line graphs, for any $k \geq 2$. Finding the required collection of regular graphs is an easy task, because the number of such graphs is usually very large, and because cospectral mates among them occur only exceptionally [2, 4, 6].

Within the proof of Theorem 1 we obtained the simple expression (5) for the energy of the second iterated line graph of a regular graph. By means of a repeated application of Eqs. (1) and (2) we could deduce analogous (yet much less simple) expressions also for $E(L^k(G))$, $k \geq 3$. In the general case, the energy of the k-th iterated line graph, $k \geq 2$, of a regular graph on n vertices and of degree $r \geq 3$ is fully determined by the parameters n and r.

References

- R. Balakrishnan, The energy of a graph, Linear Algebra Appl. 387 (2004) 287–295.
- [2] F. C. Bussemaker, S. Čobeljić, D. Cvetković, J. J. Seidel, Cubic graphs on ≤ 14 vertices, J. Combin. Theory 23B (1977) 234–235.
- [3] G. Caporossi, D. Cvetković, I. Gutman, P. Hansen, Variable neighborhood search for extremal graphs. 2. Finding graphs with extremal energy, J. Chem. Inf. Comput. Sci. 39 (1999) 984–996.
- [4] D. Cvetković, Some supplements to the tables of graph spectra, Publ. Elektrotehn. Fak. (Beograd) Ser. Mat. 7 (1996) 45–54.
- [5] D. Cvetković, M. Doob, H. Sachs, Spectra of Graphs Theory and Application, Academic Press, New York, 1980; 2nd revised ed.: Barth, Heidelberg, 1995.
- [6] D. Cvetković, M. Petrić, Tables of graph spectra, Publ. Elektrotehn. Fak. (Beograd) Ser. Mat. 4 (1993) 49–67.
- [7] H. Fripertinger, I. Gutman, A. Kerber, A. Kohnert, D. Vidović, The energy of a graph and its size dependence. An improved Monte Carlo approach, Z. Naturforsch. 56a (2001) 342–346.
- [8] A. Graovac, I. Gutman, P. E. John, D. Vidović, I. Vlah, On statistics of graph energy, Z. Naturforsch. 56a (2001) 307–311.
- [9] I. Gutman, The energy of a graph, Ber. Math. Statist. Sekt. Forschungszenturm Graz 103 (1978) 1–22.
- [10] 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.
- [11] I. Gutman, Y. Hou, Bipartite unicyclic graphs with greatest energy, MATCH Commun. Math. Comput. Chem. 43 (2001) 17–28.
- [12] I. Gutman, L. Pavlović, The energy of some graphs with large number of edges, Bull. Acad. Serbe Sci. Arts (Cl. Math. Natur.) 118 (1999) 35–50.

- [13] I. Gutman, O. E. Polansky, Mathematical Concepts in Organic Chemistry, Springer-Verlag, Berlin, 1986.
- [14] F. Harary, Graph Theory, Addison-Wesley, Reading, 1969, Chapter 8.
- [15] Y. Hou, Unicyclic graphs with minimal energy, J. Math. Chem. 29 (2001) 163–168.
- [16] Y. Hou, Bicyclic graphs with minimum energy, Linear and Multilinear Algebra 49 (2002) 347–354.
- [17] Y. Hou, I. Gutman, Hyperenergetic line graphs, MATCH Commun. Math. Comput. Chem. 43 (2001) 29–39.
- [18] Y. Hou, I. Gutman, C. W. Woo, Unicyclic graphs with maximal energy, Linear Algebra Appl. 356 (2002) 27–36.
- [19] J. Koolen, V. Moulton, Maximal energy graphs, Adv. Appl. Math. 26 (2001) 47–52.
- [20] J. Koolen, V. Moulton, Maximal energy bipartite graphs, Graphs Combin. 19 (2003) 131–135.
- [21] J. Li, X. Wang, Lower bound on the sum of positive eigenvalues of a graph, Acta Appl. Math. 14 (1998) 443–446.
- [22] D. A. Morales, Bounds for the total π-electron energy, Int. J. Quantum Chem. 88 (2002) 317–330.
- [23] D. A. Morales, Systematic search of bounds for total π-electron energy, Int. J. Quantum Chem. 93 (2003) 20–31.
- [24] H. Sachs, Über Teiler, Faktoren und charakteristische Polynome von Graphen, Teil II, Wiss. Z. TH Ilmenau 13 (1967) 405–412.
- [25] H. B. Walikar, I. Gutman, P. R. Hampiholi, H. S. Ramane, Non-hyperenergetic graphs, Graph Theory Notes New York 51 (2001) 14–16.
- [26] H. B. Walikar, H. S. Ramane, Energy of some cluster graphs, Kragujevac J. Sci. 23 (2001) 51–62.
- [27] H. B. Walikar, H. S. Ramane, Energy of some bipartite cluster graphs, Kragujevac J. Sci. 23 (2001) 63–74.

- [28] H. B. Walikar, H. S. Ramane, P. R. Hampiholi, On the energy of a graph, in: R. Balakrishnan, H. M. Mulder, A. Vijayakumar (Eds.), Graph Connections, Allied Publishers, New Delhi, 1999, pp. 120–123.
- [29] F. Zhang, H. Li, On acyclic conjugated molecules with minimal energies, Discrete Appl. Math. 92 (1999) 71–84.
- [30] F. Zhang, H. Li, On maximal energy ordering of acyclic conjugated molecules, in: P. Hansen, P. Fowler, M. Zheng (Eds.), Discrete Mathematical Chemistry, Am. Math. Soc., Providence, 2000, pp. 385–392.
- [31] F. Zhang, Z. Li, L. Wang, Hexagonal chains with maximal total π-electron energy, Chem. Phys. Lett. 337 (2001) 131–137.
- [32] F. Zhang, Z. Li, L. Wang, Hexagonal chains with minimal total π-electron energy, Chem. Phys. Lett. 337 (2001) 125–130.
- [33] B. Zhou, Energy of a graph, MATCH Commun. Math. Comput. Chem. 51 (2004) 111–118.