Faculty of Sciences and Mathematics, University of Niš, Serbia
Available at: http://www.pmf.ni.ac.rs/filomat

Filomat **23:3** (2009), 243–249 DOI:10.2298/FIL0903243S

ON THE ORIENTED INCIDENCE ENERGY AND DECOMPOSABLE GRAPHS*

Dragan Stevanović, Nair M.M. de Abreu, Maria A.A. de Freitas
Cybele Vinagre and Renata Del-Vecchio

Abstract

Let G be a simple graph with n vertices and m edges. Let edges of G be given an arbitrary orientation, and let Q be the vertex-edge incidence matrix of such oriented graph. The oriented incidence energy of G is then the sum of singular values of Q. We show that for any $n \in N$, there exists a set of n graphs with $O(n)$ vertices having equal oriented incidence energy.

1 Introduction

Let $G = (V, E)$ be a finite, simple, undirected graph with vertices $V = \{1, 2, \ldots, n\}$ and $m = |E|$ edges. Let G have adjacency matrix A with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. The energy of G was defined by Gutman in [1] as

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

and it has a long known chemical applications; for details see the surveys [2, 3, 4]. Recently, Nikiforov [5] generalized a concept of graph energy to arbitrary matrix M by defining the energy $E(M)$ to be the sum of singular values of M. The singular values of a real (not necessarily square) matrix M are the square roots of the eigenvalues of the (square) matrix MM^T, where M^T denotes the transpose of M.

Let edges of G be given an arbitrary orientation producing an oriented graph $\overrightarrow{G}$, and let Q be the vertex-edge incidence matrix of $\overrightarrow{G}$, whose (v, e) entry is equal to $+1$ if the vertex v is the head of the oriented edge e, -1 if v is the tail of e, and 0 otherwise. Then $QQ^T = L = D - A$ is the Laplacian matrix of G, where

*This work was supported by the research grant 144015G of Serbian Ministry of Science and in part by Grant 300563/94-9 of National Research Council of Brazil..
2000 *Mathematics Subject Classifications.* 05C50.
Key words and Phrases. Laplacian-like energy, Incidence energy, Decomposable graphs.
Received: October 20, 2009
Communicated by Dragan Stevanović

D is the diagonal matrix of vertex degrees [6, 7]. Suppose that L has eigenvalues $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$. The oriented incidence energy of G is then

$$OIE(G) = E(Q) = \sum_{i=1}^{n} \sqrt{\mu_i},$$

as observed in [8]. This invariant was introduced recently by Liu and Liu [9] under the name *the Laplacian energy-like invariant* and notation $LEL(G)$.

Due to its definition, it comes as no surprise that $OIE(G)$ has a number of properties analogous to $E(G)$ [9, 10]. $OIE(G)$ was suggested as a new molecular descriptor in [11]: a correlating study of OIE and topological indices provided by TOPOCLUJ software package [12], on thirteen properties of octanes, revealed that OIE describes well the properties which are well accounted by the Wiener-based molecular descriptors: octane number MON, entropy S, volume MV, or refraction MR, particularly the AF parameter, but also more difficult properties like boiling point BP, melting point MP and logP. In a second set of polycyclic aromatic hydrocarbons, OIE was proved to be as good as the Randić index and better than the Wiener index in correlations to BP, MP and logP.

A graph is *decomposable* if it can be contructed from isolated vertices by the operations of union and complement. The Laplacian spectrum of $G_1 \cup \cdots \cup G_k$ is the union of Laplacian spectra of $G_1, \ldots, G_k$, while the Laplacian spectrum of the complement of n-vertex graph G consists of values $n - \mu$, for each Laplacian eigenvalue μ of G, except for a single instance of eigenvalue 0 of G. Since the Laplacian spectrum of an isolated vertex consists of single eigenvalue 0, it is easy to conclude that the Laplacian spectrum of every decomposable graph consists of integers only [13, 14].

Much work on graph energy has appeared in literature, especially in the last decade, and a good deal of it studies graphs with equal energy [15]-[24]. Two graphs G_1 and G_2 of the same order, noncospectral with respect to L, are said to be *OIE-equienergetic* if $OIE(G_1) = OIE(G_2)$. Three pairs of connected OIE-equienergetic graphs were presented in [25] and, based on the computer search among small graphs, it was suggested that OIE-equienergetic graphs occur relatively rarely. However, note that the graphs G_{802}, G_{804} and G_{1202} from [25] are all decomposable graphs. Our goal here is to show that, for any given $n \in N$, there exists a set of n mutually OIE-equienergetic decomposable graphs with $O(n)$ vertices.

Let $A = \{a_1, \ldots, a_k\}$ be a multiset of positive integers such that $a_i \geq 3$, $i = 1, \ldots, k$. The graph S_A^*, formed from the union of stars S_{a_1-1}, S_{a_2-1}, …, S_{a_k-1} by adding a vertex adjacent to all other vertices, has $n = \left(\sum_{i=1}^{k} a_i\right) - k + 1$ vertices and $m = 2n - k - 2$ edges. It is decomposable since it can be represented as

$$S_A^* = \overline{K_1 \cup \overline{\bigcup_{i=1}^{k} \overline{K_1 \cup \overline{\overline{a_{i-2}K_1}}}}}$$

and its Laplacian spectrum is given by

$$[n, a_1, \ldots, a_k, 2^{n-2k-1}, 1^{k-1}, 0],$$

where exponents denote multiplicities. Thus,

$$OIE(S_A^*) = \sqrt{n} + \sum_{i=1}^{k} \sqrt{a_i} + (n-2k-1)\sqrt{2} + k - 1. \tag{2}$$

Let $\mathcal{S}$ be the set of of finite multisets of positive integers each of which is at least three. Let ρ be an equivalence relation on $\mathcal{S}$ defined by

$$A\,\rho\,B \quad \Leftrightarrow \quad |A| = |B|, \sum_{i=1}^{k} a_i = \sum_{i=1}^{k} b_i \text{ and } \sum_{i=1}^{k} \sqrt{a_i} = \sum_{i=1}^{k} \sqrt{b_i}.$$

From (2) we see that

$$A\,\rho\,B \quad \Rightarrow \quad OIE(S_A^*) = OIE(S_B^*).$$

Moreover, if A and B are distinct equivalent multisets, then the graphs S_A^* and S_B^* are noncospectral, while they have the same order and size.

Therefore, in order to construct sets of OIE-equienergetic decomposable graphs, we need to find nontrivial equivalence classes of ρ in $\mathcal{S}$. Construction of equivalence classes containing pairs of triplets is given in Section 2, while operations for constructing large equivalence classes in $\mathcal{S}/\rho$ are discussed in Section 3. A few nontrivial equivalence classes found by initial computer search are given in Table 1.

$\sum_i a_i = \sum_i b_i$	$\{a_1, \ldots, a_k\}$	$\{b_1, \ldots, b_k\}$	$\sum_i \sqrt{a_i} = \sum_i \sqrt{b_i}$
37	{25,6,6}	{24,9,4}	$5 + 2\sqrt{6}$
40	{27,9,4}	{25,12,3}	$5 + 3\sqrt{3}$
24	{12,4,4,4}	{9,9,3,3}	$6 + 2\sqrt{3}$
42	{20,9,9,4}	{16,16,5,5}	$8 + 2\sqrt{5}$
43	{27,4,4,4,4}	{25,9,3,3,3}	$8 + 3\sqrt{3}$

Table 1: A few equivalence classes in $\mathcal{S}$.

2 Equivalence classes containing triplets

Proposition 1. *Let a, b, c, d, e, f be positive integers such that $abc = def$. Then*

$$\{a^2c, b^2c, (d+e)^2 f\} \;\rho\; \{(a+b)^2 c, d^2 f, e^2 f\}.$$

Proof. Both multisets have three elements and the sum of square roots of their elements is equal to $(a+b)\sqrt{c}+(d+e)\sqrt{f}$. From $abc=def$ it follows that the sum of their elements are also equal,

$$(a^2+b^2)c+(d^2+e^2)f+2def=(a^2+b^2)c+2abc+(d^2+e^2)f,$$

so that these two triplets belong to the same equivalence class of ρ. ∎

For example, the first pair of triplets in Table 1 is obtained by setting $(a,b,c,d,e,f)=(1,1,6,2,3,1)$, while the second pair of triplets is obtained for $(a,b,c,d,e,f)=(2,3,1,2,1,3)$. We can construct infinitely many new pairs of triplets from Proposition 1 by taking distinct factorizations of positive integers into three factors a,b,c and d,e,f. For example, 10 can be factorized in distinct ways as

$$10=2\cdot 5\cdot 1=1\cdot 1\cdot 10,$$

which gives a new pair of equivalent triplets

$$(4,25,40) \text{ and } (49,10,10).$$

Previous proposition can be easily generalized:

Proposition 2. *For a given $k\in N$, let a_i,b_i,c_i,d_i,e_i,f_i be positive integers such that*

$$\sum_{i=1}^{k} a_ib_ic_i=\sum_{i=1}^{k} d_ie_if_i.$$

Then the multisets

$$A=\{a_i^2c_i, b_i^2c_i, (d_i+e_i)^2f_i\colon i=1,\ldots,k\}$$

and

$$B=\{(a_i+b_i)^2c_i, d_i^2f_i, e_i^2f_i\colon i=1,\ldots,k\}$$

belong to the same equivalence class of ρ.

Proof. Both A and B have $3k$ elements and the sum of square roots of their elements is equal to $\sum_{i=1}^{k}(a_i+b_i)c_i+(d_i+e_i)f_i$. For the sum of elements of A and B, we have

$$\begin{aligned}\sum_{x\in A} x &= \sum_{i=1}^{k}(a_i^2+b_i^2)c_i+(d_i^2+e_i^2)f_i+2d_ie_if_i\\ &= \sum_{i=1}^{k}(a_i^2+b_i^2)c_i+(d_i^2+e_i^2)f_i+2a_ib_ic_i=\sum_{y\in B} y. \qquad \blacksquare\end{aligned}$$

This proposition has even more freedom than Proposition 1. For example, 10 can be written in distinct ways as

$$10=1\cdot 1\cdot 4+2\cdot 3\cdot 1=1\cdot 1\cdot 5+1\cdot 1\cdot 5,$$

yielding $(a_1,b_1,c_1,a_2,b_2,c_2)=(1,1,4,2,3,1)$ and $(d_1,e_1,f_1,d_2,e_2,f_2)=(1,1,5,1,1,5)$. Proposition 2 now gives equivalent multisets

$$\{4,4,20,4,9,20\} \quad\text{and}\quad \{16,5,5,25,5,5\}.$$

3 Operations in $\mathcal{S}/\rho$

We can introduce two operations to $\mathcal{S}$ which agree with ρ to construct equivalence classes with more than two multisets. First, declare *scalar* to be a positive integer. Then for scalar α and multiset $A \in \mathcal{S}$, the product αA is defined as

$$\alpha A = \{\alpha a \colon a \in A\}.$$

The second operation is the union $A \uplus B$ of multisets A and B, which preserves multiplicities of their elements: if a appears m times in A and n times in B, then a appears $m + n$ times in $A \cup B$.

Proposition 3. *For any $\alpha \in N$ and $A, B, C, D \in \mathcal{S}$,*

$$\begin{aligned} A \ \rho \ B \quad &\Rightarrow \quad \alpha A \ \rho \ \alpha B, \\ A \ \rho \ B, C \ \rho \ D \quad &\Rightarrow \quad A \uplus C \ \rho \ B \uplus D. \end{aligned}$$

Proof. The sum of elements in αA is α times the sum of elements in A. Similarly, the sum of square roots of elements in αA is $\sqrt{\alpha}$ times the sum of square roots of elements in A. Thus, from $A \ \rho \ B$ it follows that $\alpha A \ \rho \ \alpha B$.

Next, we have

$$\sum_{x \in A \uplus C} x = \sum_{x \in A} x + \sum_{x \in C} x = \sum_{x \in B} x + \sum_{x \in D} x = \sum_{x \in B \uplus D} x,$$

and, similarly,

$$\sum_{x \in A \uplus C} \sqrt{x} = \sum_{x \in A} \sqrt{x} + \sum_{x \in C} \sqrt{x} = \sum_{x \in B} \sqrt{x} + \sum_{x \in D} \sqrt{x} = \sum_{x \in B \uplus D} \sqrt{x}.$$

Thus, $A \uplus C \ \rho \ B \uplus D$. ∎

These two operations now provide a simple way to create arbitrarily large equivalence classes. Namely, for any $A \ \rho \ B$, $n \in N$ and $\alpha_1, \ldots \alpha_n \in N$, it follows from Proposition 3 that

$$\begin{aligned} & \alpha_1 A \uplus \alpha_2 A \uplus \cdots \uplus \alpha_{n-1} A \uplus \alpha_n A \\ \rho \quad & \alpha_1 B \uplus \alpha_2 A \uplus \cdots \uplus \alpha_{n-1} A \uplus \alpha_n A \\ \rho \quad & \alpha_1 B \uplus \alpha_2 B \uplus \cdots \uplus \alpha_{n-1} A \uplus \alpha_n A \\ \rho \quad & \ldots \\ \rho \quad & \alpha_1 B \uplus \alpha_2 B \uplus \cdots \uplus \alpha_{n-1} B \uplus \alpha_n A \\ \rho \quad & \alpha_1 B \uplus \alpha_2 B \uplus \cdots \uplus \alpha_{n-1} B \uplus \alpha_n B. \end{aligned}$$

Thus, this equivalence class contains at least $n+1$ multisets, each of them containing $n|A|$ elements.

In particular, take $A = \{25, 6, 6\}$, $B = \{24, 9, 4\}$ and $\alpha_1 = \cdots = \alpha_n = 1$. Then for any $n \in N$, we have a set of $n+1$ OIE-equienergetic noncospectral decomposable graphs

$$S^*_{A \uplus A \uplus \cdots \uplus A}, S^*_{B \uplus A \uplus \cdots \uplus A}, S^*_{B \uplus B \uplus \cdots \uplus A}, \ldots, S^*_{B \uplus B \uplus \cdots \uplus B},$$

each of which has $34n + 1$ vertices and $65n$ edges.

4 Concluding remarks

Our last example shows that for any $n \in N$, there exists a set of n OIE-equienergetic noncospectral graphs with $O(n)$ vertices. Propositions 1, 2 and 3 provide means to construct an abundance of further examples of OIE-equienergetic noncospectral graphs. It should be noted, however, that all these graphs have more vertices than what can be reached by a computer search on modern day computers, so that our finding, in fact, should not be considered contradictory to the conclusion from [25] that OIE-equienergetic graphs occur relatively rarely.

References

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

[2] I. Gutman, *Total π-electron energy of benzenoid hydrocarbons*, Topics Curr. Chem. 162 (1992), 29–63.

[3] 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.

[4] 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.

[5] V. Nikiforov, *The energy of graphs and matrices*, J. Math. Anal. Appl. 326 (2007), 1472–1475.

[6] R. Merris, *Laplacian matrices of graphs: A survey*, Linear Algebra Appl. 197–198 (1994), 143–176.

[7] R. Merris, *A survey of graph Laplacians*, Linear Multilin. Algebra 39 (1995), 19–31.

[8] I. Gutman, D. Kiani, M. Mirzakhah, B. Zhou, *On Incidence Energy of a Graph*, Linear Algebra Appl, to appear.

[9] J. Liu, B. Liu, *A Laplacian-Energy-Like Invariant of a Graph*, MATCH Commun. Math. Comput. Chem. 59 (2008), 355–372.

[10] D. Stevanović, *Laplacian-like energy of trees*, MATCH Commun. Math. Comput. Chem. 61 (2009), 407–417.

[11] D. Stevanović, A. Ilić, C. Onisor, M.V. Diudea, *LEL—a newly designed molecular descriptor*, Acta Chim. Slov. 56 (2009), 410–417.

[12] O. Ursu, M.V. Diudea, TOPOCLUJ 4.0, Babes-Bolyai University, 2005.

[13] S. Kirkland, *Constructably Laplacian integral graphs*, Linear Algebra Appl. 423 (2007), 3–21.

[14] R. Grone, R. Merris, *Indecomposable Laplacian integral graphs*, Linear Algebra Appl. 428 (2008), 1565–1570.

[15] V. Brankov, D. Stevanović, I. Gutman, *Equienergetic chemical trees*, J. Serb. Chem. Soc. 69 (2004), 549–554.

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

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

[18] D. Stevanović, *Energy and NEPS of graphs*, Linear Multilinear Algebra 53 (2005), 67–74.

[19] 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.

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

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

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

[23] G. Indulal, A. Vijayakumar, *A Note on Energy of Some Graphs*, MATCH Commun. Math. Comput. Chem. 59 (2008), 269–274.

[24] J. Liu, B. Liu, *Note on a Pair of Equienergetic Graphs*, MATCH Commun. Math. Comput. Chem. 59 (2008), 275–278.

[25] J. Liu, B. Liu, S. Radenković, I. Gutman, *Minimal LEL-equienergetic graphs*, MATCH Commun. Math. Comput. Chem. 61 (2009), 471–478.

University of Niš, Faculty of Science and Mathematics, Višegradska 33, 18000 Niš, Serbia
Federal University of Rio de Janeiro, Brazil, Production Engineering Program, COPPE, Bloco F, Ilha do Fundão, Rio de Janeiro, Brazil
Fluminense Federal University, Mathematical Institute, Praça do Valonguinho, Centro, Niterói, Brazil

E-mails: dragance106@yahoo.com (D. Stevanović),
nair@pep.ufrj.br (N.M.M. de Abreu),
maguieiras@im.ufrj.br (M.A.A. de Freitas),
cybl@vm.uff.br (C. Vinagre),
renata@vm.uff.br (R. Del-Vecchio)