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GRAPH ENERGIES AND THEIR APPLICATIONS

IVAN GUTMAN, BORIS FURTULA

(Presented at the 6th Meeting, held on September 27, 2019)

A b s t r a c t. The energy $E(G)$ of a graph G is the sum of absolute values of the eigenvalues of the adjacency matrix of G. This spectral quantity was introduced in 1978 by Ivan Gutman, but its extensive research started only twenty five years later. A large number (over hundred) variants of graph energy have been proposed, based on matrices other than the adjacency matrix. Research of these graph energies is nowadays very active, resulting in well over a thousand publications. In recent years, more than two papers on graph energies appear each week. Graph energies found a remarkable number of various applications. In this paper, we outline some basic, mainly statistical, facts on the research of graph energies, and point out their main applications.

AMS Mathematics Subject Classification (2010): 05C50, 05C90.

Key Words: energy (of graph), spectrum (of graph), spectrum (of matrix), singular value (of matrix).

1. *Introduction*

In 1978 one of the present authors (I.G.) introduced a novel graph spectral quantity which he named *graph energy* [1].

Let G be a simple graph of order n. Let $\mathbf{A}(G)$ be its adjacency matrix. The eigenvalues of $\mathbf{A}(G)$, denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$, form the spectrum of G [2].

Definition 1.1. (Gutman, 1978, [1]) The energy of the graph G is

$$E(G) = \sum_{i=1}^{n} |\lambda_i| \,. \tag{1.1}$$

This definition was motivated by several earlier known results for the Hückel molecular orbital total π-electron energy [3–5]. The author of Definition 1.1 put forward it in good hope that the mathematical community will recognize its significance, and that it will trigger future research and lead to the discovery of numerous additional results. What happened was a lack of any interest for the graph energy concept, in spite of the author's several attempts to popularize it [6–10]. In the next more than twenty years, the graph energy concept was almost completely ignored by other mathematicians. Then, somewhere after year 2000 a fortunate change happened. Suddenly, several mutually unrelated mathematicians started to examine graph energy and publish papers on it. What followed was an almost explosive growth in interest for graph energy, in practically every part of the globe, resulting in a large number of publications. In the recent years, more than two papers on graph energy are published each week.

Research of graph energy and its numerous variants shows no sign of attenuation. On the other hand, the time of I.G. is about to expire. In view of this, we found it purposeful to present data on the enormous increase of work in this area. In addition, we outline the various, sometimes quite unexpected and surprising, applications that graph energies have found in other fields of science.

The data given in the present article are those that we collected by May 1, 2019.

2. *Graph energy and its variants*

Let, as before, G be a graph of order n, and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of its adjacency matrix. Assume that these are labeled in a non-increasing order. Then, within the Hückel molecular orbital theory, the total energy of π-electrons of an unsaturated conjugated hydrocarbon is given by [12]

$$E_\pi = \begin{cases} 2\sum\limits_{i=1}^{n/2} \lambda_i & \text{if } n \text{ is even,} \\[2ex] 2\sum\limits_{i=1}^{(n-1)/2} \lambda_i + \lambda_{(n+1)/2} & \text{if } n \text{ is odd}\,. \end{cases} \tag{2.1}$$

Note that the graph G to which Eq. (2.1) is applicable, the so-called "molecular graph", must satisfy several structural limitations. For instance, G must be connected and its maximum vertex degree is at most 3. It was to be expected that mathematicians will not be particularly interested to study an awkward graph-spectral quantity such as the right–hand side of Eq. (2.1), which anyway would be applicable to a narrow class of graphs.

On the other hand, it could be easily shown that if the conditions

$$\begin{aligned} &\lambda_{n/2} \geq 0 \geq \lambda_{n/2+1} && \text{if } n \text{ is even,} \\ &\lambda_{(n+1)/2} = 0 && \text{if } n \text{ is odd}\,. \end{aligned} \tag{2.2}$$

are satisfied, then Eq. (2.1) reduces to

$$E_\pi = \sum_{i=1}^{n} |\lambda_i|\,.$$

This observation led directly to the idea to define graph energy via Eq. (1.1).

Details on the validity of conditions (2.2), as well on other mathematical arguments in favor of Eq. (1.1) can be found elsewhere [11, 13, 14].

After a quarter-of-century delay, an extensive research of graph energy started, and is still vigorous. The main results achieved in this area are presented in the book [13].

Motivated by the success of the theory of graph energy, its variants were proposed, based on matrices other than the adjacency matrix. In what follows we define the first few such graph energies.

Denote by $\deg(i)$ the degree of the i-th vertex of the graph G. Let $\mathbf{\Delta}(G)$ be the diagonal matrix of vertex degrees. Then the *Laplacian matrix* of G is

$$\mathbf{L}(G) = \mathbf{\Delta}(G) - \mathbf{A}(G).$$

The *extended adjacency matrix* is the square matrix of order n, whose (i, j)-element is equal to

$$\frac{1}{2}\left(\frac{\deg(i)}{\deg(j)} + \frac{\deg(j)}{\deg(i)}\right)$$

if i and j are adjacent vertices, and is zero otherwise [15]. The *Randić matrix* of the graph G is the square matrix of order n, whose (i, j)-element is equal to

$$\frac{1}{\sqrt{\deg(i)\ \deg(j)}}$$

if i and j are adjacent vertices, and is zero otherwise [16]. The *distance matrix* of a connected graph G is the square matrix of order n whose (i, j)-element is the distance between the vertices i and j.

Definition 2.1. (a) The extended energy is the sum of absolute values of the eigenvalues of the extended adjacency matrix [15].

(b) The Laplacian energy of a graph of order n and size m is the sum of absolute values of the eigenvalues of $\mathbf{L}(G) - \frac{2m}{n}\,\mathbf{I}_n$, where $\mathbf{I}_n$ is the unit matrix of order n [17].

(c) The distance energy of a connected graph is the sum of absolute values of the eigenvalues of the distance matrix [18].

(d) The Randić energy is the sum of absolute values of the eigenvalues of the Randić matrix [16].

Let $\mathbf{M}$ be a matrix of dimension $p \times q$, and let $\mathbf{M}^t$ be its inverse. Then the singular values of $\mathbf{M}$ are the positive square roots of the eigenvalues of $\mathbf{M}\,\mathbf{M}^t$.

A significant step forward in the theory of graph energy was made by Vladimir Nikiforov [19].

Definition 2.2. (Nikiforov, 2007, [19]) Let $\sigma_1, \sigma_2, \ldots, \sigma_p$ be the singular values of the matrix $\mathbf{M}$. Then the energy of $\mathbf{M}$ is

$$E(\mathbf{M}) = \sum_{i=1}^{p} \sigma_i \,.$$

Needless to say that in the case of square symmetric matrices, the energies defined in Definitions 1.1, 2.1, and 2.2 coincide.

3. *Expansion of research of graph energies*

In recent years a plethora of other graph energies appeared in the literature. We list here only their names, whereas more details and the respective references can be found in the book [11]. At the present moment, this list consists of over hundred graph energies, and more will, for sure, appear in the future. Thus, in addition to extended, distance, Laplacian, and Randić energies, we have:

ABC energy
accurate independent dominating energy
additive color Laplacian energy
Albertson energy
arithmetic–geometric energy
average degree energy
average degree-eccentricity energy
color energy

color Laplacian energy
color signless Laplacian energy
common-neighborhood energy
complement Randić energy
complementary distance energy
complementary distance signless Laplacian energy
complementary dominating energy
connected complement domination energy
Co-PI energy
Coxeter energy
degree equitable connected cototal dominating energy
degree product energy
degree subtraction energy
degree subtraction adjacency energy
degree sum energy
detour energy
distance signless Laplacian energy
domination energy
double dominating energy
e-energy
eccentric Laplacian energy
edge energy
edge-Zagreb energy
extended ABC energy
extended signless Laplacian energy
first Hermitian–Zagreb energy
forgotten energy
general Randić energy
general sum-connectivity energy
geometric–arithmetic energy
greatest common divisor energy
greatest common divisor degree energy
Harary energy
harmonic energy
He energy
Hermitian energy
Hermitian–Randić energy

incidence energy
intrinsic energy
inverse dominating energy
inverse sum indeg energy
iota energy
Kirchhoff energy
Laplacian distance energy
Laplacian incidence energy
Laplacian minimum boundary dominating energy
Laplacian minimum-covering energy
Laplacian minimum-covering chromatic energy
Laplacian minimum-covering color energy
Laplacian minimum dominating energy
Laplacian partition energy
Laplacian resolvent energy
Laplacian sum-eccentricity energy
matching energy
maximum degree energy
maximum eccentricity energy
maximum independent vertex energy
minimum boundary dominating energy
minimum-covering energy
minimum-covering color energy
minimum-covering distance energy
minimum-covering Gutman energy
minimum-covering Harary energy
minimum-covering Randić energy
minimum-covering reciprocal distance signless Laplacian energy
minimum-covering Seidel energy
minimum-domination energy
minimum *bb*-dominating energy
minimum dom strong dominating energy
minimum-dominating distance energy
minimum-dominating Harary energy
minimum-dominating maximum degree energy
minimum-dominating partition energy
minimum-dominating Randić energy

minimum-dominating Seidel energy
minimum edge covering energy
minimum edge dominating energy
minimum efficient dominating energy
minimum equitable color dominating energy
minimum equitable dominating energy
minimum equitable dominating Randić energy
minimum hub energy
minimum hub distance energy
minimum Laplacian efficient dominating energy
minimum majority domination energy
minimum-maximal-domination energy
minimum mean boundary dominating energy
minimum mean dominating energy
minimum mean dominating distance energy
minimum monopoly energy
minimum monopoly distance energy
minimum neighborhood energy
minimum paired dominating energy
minimum robust domination energy
minimum total edge dominating energy
n-energy
net-Laplacian energy
non-common neighborhood energy
normalized incidence energy
normalized Laplacian energy
normalized Laplacian resolvent energy
o-energy
oriented incidence energy
partition energy
path energy
path Laplacian energy
peripheral distance energy
PI energy
Randić color energy
Randić incidence energy
rational metric energy

reciprocal complementary distance energy
reciprocal distance signless Laplacian energy
reciprocal Randić energy
reciprocal sum-connectivity energy
reduced color energies (two)
resistance-distance energy
resolvent energy
second–stage energy
Seidel energy
Seidel Laplacian energy
Seidel signless Laplacian energy
signless Laplacian energy
signless Laplacian resolvent energy
skew energy
skew Randić energy
skew Laplacian energy
so-energy
sum-connectivity energy
sum-eccentricity energy
symmetric division deg energy
Szeged energy
terminal distance energy
total digraph energy
ultimate energy
upper dominating energy
vertex energy
vertex degree energy
vertex Zagreb adjacency energy
Zagreb energies (two)
α-distance energy
α-incidence energy

The graph energy concept was extended also to polynomials, semigroups, and matroids.

The extent of research on graph energies, and its change over time, can be seen from Table 1 and Figure 1. In our records, we have references to over 1100 published papers (which do not include Ph.D. and M.Sc. theses, conference reports, or preliminary announcements); these can be found in the book [11].

year	#pap.	comment	year	#pap.	comment
1996	2		2008	56	$>$ o.p.w.
1997	0		2009	72	$>$ o.p.w.
1998	2		2010	69	$>$ o.p.w.
1999	6		2011	61	$>$ o.p.w.
2000	4		2012	63	$>$ o.p.w.
2001	12		2013	63	$>$ o.p.w.
2002	3		2014	76	$>$ o.p.w.
2003	5		2015	114	$>$ t.p.w.
2004	9		2016	113	$>$ t.p.w.
2005	16		2017	132	$>$ t.p.w.
2006	11		2018	113	$>$ t.p.w.
2007	35		2019	63	as on May 1

Table 1: Number of published works on graph energies that appeared around year 2000 and later. In the last few years, such papers were produced faster than one per week (= o.p.w.) or two per week (= t.p.w.). Attenuation of this speed is not to be expected in the foreseen future. The authors are aware that there must be numerous additional papers published in India and China (in particular, those in Chinese language) that are not accounted for.

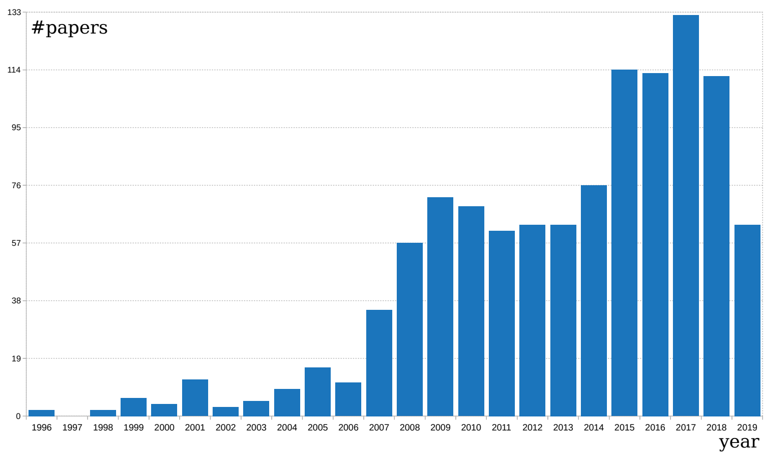

Figure 1: Distribution of the published graph energy papers by years.

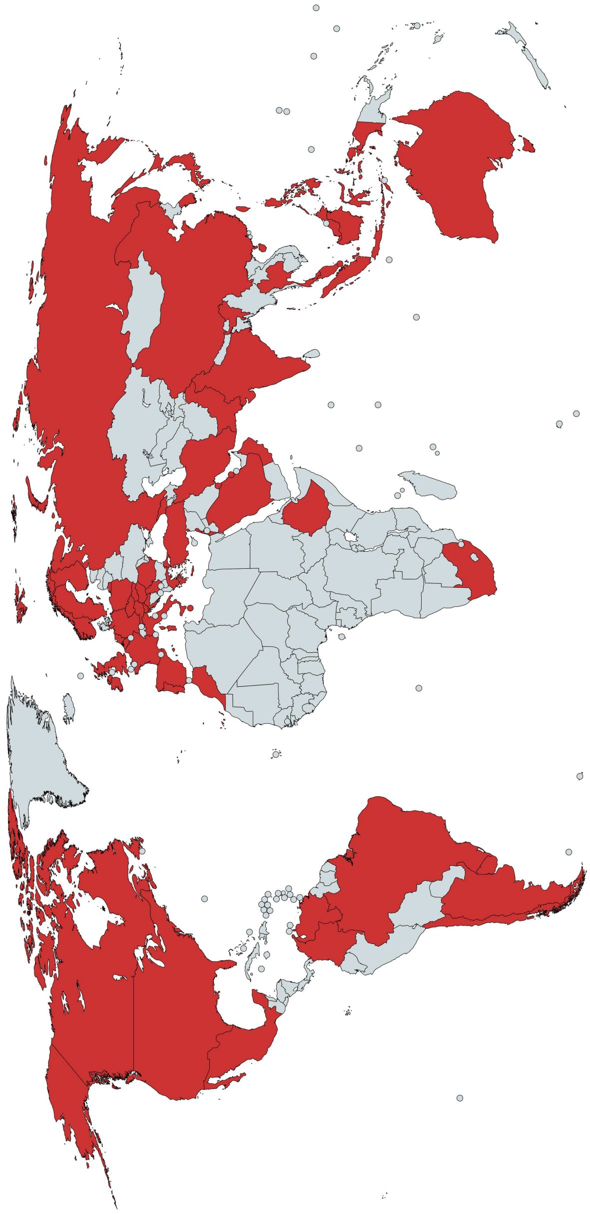

Figure 2: Parts of the world in which researches of graph energies have been conducted.

Research of graph energies is conducted literally all over the world. Table 2 and Figure 2 show the distribution of authors of graph-energy-papers by the country of affiliations.

country	no.	country	no.	country	no.	country	no.
Argentina	6	Georgia	1	Mexico	7	Slovenia	4
Australia	6	Germany	11	Morocco	1	South Africa	5
Austria	3	Greece	2	Norway	1	South Korea	15
Bahrain	1	Hungary	2	Netherlands	5	Spain	2
Belgium	2	India	260	Oman	4	Sweden	1
Brazil	16	Indonesia	8	Pakistan	25	Taiwan	4
Canada	9	Iran	89	Philippines	3	Thailand	3
Chile	16	Ireland	1	Poland	3	Turkey	23
China	267	Israel	1	Portugal	3	UK	10
Colombia	12	Italy	15	Romania	5	Uruguay	2
Croatia	4	Japan	4	Russia	1	USA	66
Czechia	1	Kuwait	7	Saudi Arabia	6	Venezuela	8
Ethiopia	1	Lebanon	1	Serbia	39		
Finland	2	Malaysia	15	Singapore	2		
France	8	Malta	4	Slovakia	2		

Table 2: Number of scholars from various countries who authored or coauthored at least one article on graph energy in the period 1996–2019 (as on May 1, 2019). Their true count is somewhat greater because we did not distinguish between scholars with the same surname and different names beginning with the same letter. Thus, Xia Li, Xuechao Li, and Xueliang Li were counted as one. Note that all continents, with the regretful exception of Antarctica, are represented in this field of research.

4. *Applications of graph energies*

Although graph energy and its later variants were introduced solely for mathematical investigations, these energies found a remarkable, somewhat surprising and mysterious, applications in other fields of science and engineering. Applications of graph energy in the chemistry of unsaturated conjugated molecules are obvious, rather numerous, and will not be further commented here. Somewhat related are applications in crystallography [20,21], theory of macromolecules [22,23], as well as analysis and comparison of protein sequences [24–27]. Also not particularly unexpected are attempts to apply graph energies in network analysis [28–35], including problems of air transportation [30], satellite communication [32], and biology [29]. Related applications in computer science and process analysis were reported in [36–39] and [40,41], respectively.

Unexpected applications of graph energies are in engineering, in complex system design and analysis [42–47]. Especially worth mentioning is their use in construction of spacecrafts [44].

Another unexpected area of application are pattern recognition and object identification [48–52]. These approaches may be of some value for military purposes. On the other hand, face recognition [52] may be of interest to police.

For the authors of this article, most pleasing was to learn that Laplacian graph energy found such an unexpected application as image analysis and processing [53–57]. The inventors of Laplacian energy [17] are especially delighted with the fact that it is used for classifying high resolution satellite images [56].

Some attempts to use graph energies in medicine have also appeared in the literature [58–62]. Less mysterious are applications to epidemics [62] and neuronal [58,61] networks. Connecting a graph-energy-like quantity to Alzheimer disease [60] sounds like science fiction. The bizarre idea of using minimum robust domination energy for "disruption of cell wall fatty acid biosynthesis in *Mycobacterium tuberculosis* " [59] is beyond our comprehension.

5. *Concluding remarks*

The concept of graph energy was proposed in 1978 by Ivan Gutman in a humble and difficult-to-find article [1]. After a latent period of about 25 years, the mathematical community recognized the value of this concept, leading to the discovery of numerous new results. A plethora (well over one hundred) of variants of graph energy has been introduced. All this resulted in a rapid growth of published papers, which nowadays exceeds two per week.

Graph energies found unexpected applications in such areas of science and engineering as crystallography, air transportation, satellite communication, face recognition, comparison of protein sequences, construction of spacecrafts, processing of high resolution satellite images. Also some applications in medicine have been attempted.

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