

## COMPARATIVE STUDY OF GRAPH ENERGIES

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*A b s t r a c t.* The ordinary energy of the graph is defined as the sum of the absolute values of the eigenvalues of its adjacency matrix. In recent times analogous “energies” are being considered, based on the eigenvalues of a variety of other graph matrices. We briefly survey and comment this “energy deluge”, and then show that some of the results obtained (one-by-one) for different graph energies, are special cases of a single general result, that is independent of any graph-theoretical interpretation.

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### 1. Introduction

The *energy* of a graph is equal to the sum of the absolute values of its eigenvalues. This concept was proposed quite some time ago in the paper [40] (and later on several other occasions). After a long latent period, it now became a popular topic of research. Details of the theory of graph

energy can be found in the reviews [43, 50, 45], as well as in the books [69, 22, 23]. Recent monographs on linear algebra and spectral graph theory [15, 114, 11, 25] contain sections devoted to graph energy.

The motivation for the study of the graph energy comes from chemistry, where the research on the so-called *total  $\pi$ -electron energy* can be traced back until the 1930s; for more details and bibliography see [35, 44, 52, 53, 42, 41].

Let  $G$  be a graph possessing  $n$  vertices and  $m$  edges. Let  $v_1, v_2, \dots, v_n$  be the vertices of  $G$ . Then the adjacency matrix  $\mathbf{A} = \mathbf{A}(G)$  of the graph  $G$  is the square matrix of order  $n$  whose  $(i, j)$  entry is defined as [21, 25]

$$a_{ij} = \begin{cases} 1 & \text{if } i \neq j, \text{ and } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & \text{if } i \neq j, \text{ and } v_i \text{ and } v_j \text{ are not adjacent} \\ 0 & \text{if } i = j . \end{cases}$$

Let  $\lambda_1, \lambda_2, \dots, \lambda_n$  be the eigenvalues of  $\mathbf{A}(G)$ . These eigenvalues are said to be the eigenvalues of the graph  $G$  and to form its spectrum [21, 25]. Then the energy of  $G$  is defined as

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

In what follows,  $E(G)$  will be referred as the *ordinary energy* of the graph  $G$ .

Since the graph energy showed to be a mathematically interesting concept, and since hundreds of non-trivial results on it could be obtained [69], the natural idea was to use eigenvalues of other graph matrices, and consider other graph energies. Since 2006, when the first such extension was put forward [54], an unexpectedly large number of graph energies appeared in the mathematical and mathematico-chemical literature. The aim of the present article is to survey and comment this “*energy deluge*” and to offer some unifying ideas.

At this point it should be noted that in the mathematical and mathematico-chemical literature there exist countless graph matrices (i. e., matrices defined in terms of certain structural details of the underlying graph) [62], and that the “invention” of more such matrices is easy and elementary.

## 2. Some non-ordinary graph energies

In this section we outline the basic results on a few non-ordinary graph energies, which – until now – have attracted the greatest attention and are considered in the greatest number of published papers.

### 2.1. Laplacian and signless Laplacian energy

The Laplacian matrix  $\mathbf{L} = \mathbf{L}(G)$  of an  $(n, m)$ -graph  $G$  is defined via its matrix elements as [25]:

$$\ell_{ij} = \begin{cases} -1 & \text{if } i \neq j, \text{ and } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & \text{if } i \neq j, \text{ and } v_i \text{ and } v_j \text{ are not adjacent} \\ d_i & \text{if } i = j \end{cases} \quad (2)$$

where  $d_i$  is the degree of the  $i$ -th vertex of  $G$ . Its eigenvalues are denoted by  $\mu_1, \mu_2, \dots, \mu_n$ .

Because  $\mu_i \geq 0$  and  $\sum_{i=1}^n \mu_i = 2m$ , it would be trivial to define the Laplacian–spectrum version of graph energy as  $\sum_{i=1}^n |\mu_i|$ . Instead, the Laplacian energy was conceived as [54]

$$LE = LE(G) := \sum_{i=1}^n \left| \mu_i - \frac{2m}{n} \right|. \quad (3)$$

This definition is adjusted so that for regular graphs,  $LE(G) = E(G)$ .

Various properties of the Laplacian energy were established in the papers [6, 27, 31, 46, 54, 67, 73, 91, 95, 96, 97, 98, 102, 108, 115, 117, 118, 119, 121, 122, 124, 30, 18, 75, 113, 32, 79, 57]. Of these we mention the conjecture [46] that for all graphs  $LE \geq E$ . This conjecture was corroborated by numerous examples [46, 91], but eventually, by means of counterexamples, was shown to be false in the general case [73, 108]. Finally, it was proven [98, 96] that  $LE(G) \geq E(G)$  holds for all bipartite graphs. Du, Li and Li [29] proved that the conjecture is true for almost all graphs (see also [28]).

The fact that for a (disconnected) graph  $G$  consisting of (disjoint) components  $G_1$  and  $G_2$ , the equality

$$LE(G) = LE(G_1) + LE(G_2) \quad (4)$$

is not generally valid, may be considered as a serious drawback of the Laplacian–energy concept [54].

The Nordhaus–Gaddum–type bounds [8] for  $LE$  read [122]:

$$2(n-1) \leq LE(G) + LE(\overline{G}) < n\sqrt{n^2-1}$$

with equality on the left-hand side if and only if  $G \cong K_n$  or  $G \cong \overline{K_n}$ .

The signless Laplacian matrix  $\mathbf{L}^+ = \mathbf{L}^+(\mathbf{G})$  is defined via

$$\ell_{ij}^+ = \begin{cases} +1 & \text{if } i \neq j, \text{ and } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & \text{if } i \neq j, \text{ and } v_i \text{ and } v_j \text{ are not adjacent} \\ d_i & \text{if } i = j \end{cases}$$

which should be compared with Eq. (2). In [98, 1] the analogue of  $LE$  was considered. Details of the theory of spectra of the signless Laplacian matrix are found in the review [24]. Let  $\mu_1^+, \mu_2^+, \dots, \mu_n^+$  be the eigenvalues of  $\mathbf{L}^+$ . Then, in analogy to Eq. (3), we define

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

Also in this case, for regular graphs,  $LE^+(G) = E(G)$ .

For bipartite graph  $LE^+ = LE$ . For non-bipartite graphs the relation between  $LE^+$  and  $LE$  is not known, but seems to be not simple. More on  $LE^+$  is found in Subsection 0.1.

## 2.2. Distance energy

Let  $G$  be a connected graph on  $n$  vertices, whose vertices are  $v_1, v_2, \dots, v_n$ . The distance matrix of  $G$  is the square matrix of order  $n$  whose  $(i, j)$ -entry is the distance (= length of the shortest path) between the vertices  $v_i$  and  $v_j$ .

Let  $\rho_1, \rho_2, \dots, \rho_n$  be the eigenvalues of the distance matrix of  $G$ . Since the sum of these eigenvalues is zero, there is no obstacle to define the distance energy as [60, 92]

$$DE = DE(G) := \sum_{i=1}^n |\rho_i|.$$

Only some elementary (and not very exciting) properties of the distance energy were established until now : bounds [14, 28, 59, 60, 93, 125, 37], examples of distance–equienergetic graphs [61, 77, 92, 94, 57], and formulas

for  $DE$  of special types of graphs [94, 107, 56, 16]. For a generalization of the distance–energy concept see [68].

### 2.3. Energy of matrices

Nikiforov [84, 85, 86] proposed a significant extension and generalization of the graph–energy concept. Let  $\mathbf{M}$  be a  $p \times q$  matrix with real–valued elements, and let  $s_1, s_2, \dots, s_p$  be its singular values. Then the energy of  $\mathbf{M}$  can be defined as [84]

$$E(\mathbf{M}) := \sum_{i=1}^p s_i . \quad (5)$$

Recall that the singular values of the (real) matrix  $\mathbf{M}$  are equal to the (positive) square roots of the eigenvalues of  $\mathbf{M}\mathbf{M}^t$ .

Formula (5) is in full harmony with the ordinary graph–energy concept. As easily seen,  $E(G) = E(\mathbf{A}(G))$ . Also,

$$LE(G) = E\left(\mathbf{L}(G) - \frac{2m}{n}\mathbf{I}\right) \quad \text{and} \quad LE^+(G) = E\left(\mathbf{L}^+(G) - \frac{2m}{n}\mathbf{I}\right).$$

By means of formula (5) an infinite number of “energies” of non-square matrices could be imagined, see Section ???. Until now only the energy of the incidence matrix (see Subsection 0.1) was studied in some detail.

### 0.1 $LEL$ and incidence energy

In order to find a Laplacian–eigenvalue based energy, in which a formula of the type (4) would be generally valid, Liu and Liu [72] proposed a “Laplacian–energy like” invariant, defined as

$$LEL = LEL(G) := \sum_{i=1}^n \sqrt{\mu_i} . \quad (6)$$

As a direct consequence of this definition, the relation

$$LEL(G) = LEL(G_1) + LEL(G_2)$$

is satisfied by any graph  $G$  whose components are  $G_1$  and  $G_2$ . On the other hand, if  $G$  is a regular graph, then  $LEL(G) = E(G)$  does not hold.

Formula (6) does not have the form of an “energy”, and therefore was initially viewed as a dead–end of the research on graph energies. Only a few results on  $LEL$  were reported [28, 58, 76, 78, 101, 105, 106, 70, 17, 128, 112,

109]. It was pointed out [55] that in spite of its dependence on Laplacian eigenvalues,  $LEL$  is more similar to  $E$  than to  $LE$ .

Independently of the research on  $LEL$ , Jooyandeh et al. [63] introduced the “incidence energy”  $IE$ , as the energy of the incidence matrix of a graph, cf. Eq. (5).

If  $G$  is a graph with vertices  $v_1, v_2, \dots, v_n$  and edges  $e_1, e_2, \dots, e_m$ , then its vertex–edge incidence matrix is an  $n \times m$  matrix whose  $(i, j)$ -entry is equal to 1 if  $v_i$  is an end-vertex of the edge  $e_j$ , and is zero otherwise.

It could be shown that [48]

$$IE(G) = \sum_{i=1}^n \sqrt{\mu_i^+}$$

which, in turn, implies that for bipartite graphs, the incidence energy is same as  $LEL$ . This finding gave a new rationale to the study of both  $LEL$  and  $IE$ .

Let  $\psi(G, \lambda)$  be the characteristic polynomial of the signless Laplacian matrix of the graph  $G$ . It is known [24] that it has the form

$$\psi(G, \lambda) = \sum_{k \geq 0} (-1)^k c_k(G) \lambda^{n-k}$$

where  $c_k(G) \geq 0$ .

Let  $\Psi(G, \lambda) = \psi(G, \lambda^2)$ . The zeros of  $\Psi(G, \lambda)$  are  $\pm\sqrt{\mu_1^+}, \pm\sqrt{\mu_2^+}, \dots, \pm\sqrt{\mu_n^+}$ . Consequently, the sum of the positive zeros of  $\Psi(G, \lambda)$  is just  $IE(G)$ .

The Coulson integral formula (see [40, 51, 81]) makes it possible to compute the sum of positive zeros of a polynomial. This yields [48]:

$$IE(G) = \frac{1}{\pi} \int_0^{+\infty} \ln \left[ \sum_{k \geq 0} c_k(G) x^{2k} \right] \frac{dx}{x^2}.$$

It is seen that  $IE$  is a monotonically increasing function of each coefficient  $c_k$ . Based on this observation, it is possible to compare the  $IE$ -values of various graphs. For instance, from the fact that [123]

$$c_k(S_n) \leq c_k(T) \leq c_k(P_n)$$

which holds for all  $n$ -vertex trees  $T$  and for all  $k \geq 0$ , it follows that the star  $S_n$  is the  $n$ -vertex tree with minimal, and the path  $P_n$  the  $n$ -vertex tree with maximal incidence energy.

Other results obtained for incidence energy and  $LEL$  can be found in the papers [49, 55, 120, 110, 5, 126, 109]. For a review on both  $LEL$  and  $IE$  see [71]. For generalizations of incidence energy see [68, 104, 103].

### 3. The energy deluge

In the general case, the eigenvalues of a digraph are complex numbers. In view of this, the definition of graph energy via Eq. (1) cannot be straightforwardly extended to digraphs. According to Rada [87, 88, 89, 36, 9, 90], the energy of a digraph  $D$  with eigenvalues  $\lambda_1, \lambda_2, \dots, \lambda_n$  can be defined as

$$E(D) := \sum_{i=1}^n |Re(\lambda_i)|$$

where  $Re(z)$  stands for the real part of the complex number  $z$ . If so, then the Coulson integral formula (see [40, 51, 81]) is applicable to  $E(D)$ .

Another approach to the energy of digraphs was followed by Kharaghani and Tayfeh-Rezaie [64], utilizing the singular values of the adjacency matrix of  $D$ . In fact, in [64] the energy of an arbitrary (square)  $(0, 1)$ -matrix was considered. Klein and Rosenfeld [65, 66] considered the energy of graphs in which an ordinary edge was replaced by two oppositely directed edges, one with weight  $exp(i\alpha)$ , the other weighted  $exp(-i\alpha)$ .

A third approach to digraphs was put forward by Adiga, Balakrishnan and So [2]. They and some other authors [111, 34] studied the *skew energy* defined as the sum of the absolute values of the eigenvalues of the skew-adjacency matrix. (Recall that the  $(i, j)$ -entry of the skew-adjacency matrix is  $+1$  if an edge is directed from the  $i$ -th vertex to the  $j$ -th vertex, in which case the  $(j, i)$ -entry is  $-1$ . If there is no directed edge between the vertices  $i$  and  $j$ , then the respective matrix element is zero.) The skew Laplacian energy of a digraph was considered in [3].

When speaking of the energy of a digraph, one must not forget that the existence of a directed cycle is a necessary condition for the existence of a nonzero eigenvalue. In other words, the energy of a digraph without directed cycles (e. g. of any directed tree) is equal to zero.

The energy of signed graphs was also examined [33].

Without being aware of the Laplacian and distance energy, Consonni and Todeschini [19] introduced a whole class of matrix-based quantities, defined as

$$\sum_{i=1}^n |x_i - \bar{x}| \tag{7}$$

where  $x_1, x_2, \dots, x_n$  are the eigenvalues of the respective matrix, and  $\bar{x}$  is their arithmetic mean. Evidently, if the underlying matrix is the adjacency, Laplacian, signless Laplacian, or distance matrix, then the quantity defined via (7) is just the ordinary graph energy, Laplacian energy, signed Laplacian energy, and distance energy, respectively. Consonni and Todeschini used the invariants defined via (7) for constructing mathematical models capable to predicting various physico-chemical properties of organic molecules. Therefore their article [19] is valuable as documenting the applicability of various “energies” in natural sciences (in particular, in chemistry).

We end this section by briefly listing other graph energies that appeared in the literature.

- The energy of a general **Hermitian matrix** was examined in [74].
- **Randić energy** [13, 99] is the energy of the Randić matrix, whose  $(i, j)$ -element is

$$R_{ij} = \begin{cases} 1/\sqrt{d_i d_j} & \text{if } i \neq j, \text{ and } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & \text{otherwise} \end{cases}$$

where  $d_i$  stands for the degree of the  $i$ -th vertex.

- **Sum-connectivity energy** [127, 116] is the energy of the matrix, whose  $(i, j)$ -element is

$$SC_{ij} = \begin{cases} 1/\sqrt{d_i + d_j} & \text{if } i \neq j, \text{ and } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & \text{otherwise .} \end{cases}$$

- **Maximum-degree energy** [4] is the energy of the matrix, whose  $(i, j)$ -element is

$$MD_{ij} = \begin{cases} \max\{d_i, d_j\} & \text{if } i \neq j, \text{ and } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & \text{otherwise .} \end{cases}$$

- **Harary energy** [38, 20] is the energy of the Harary matrix, whose  $(i, j)$ -element is

$$H_{ij} = \begin{cases} 1/d(v_i, v_j) & \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases}$$

where  $d(v_i, v_j)$  stands for the distance between the vertices  $v_i$  and  $v_j$ .



- **PI and vertex-PI energy** [83] are the energies of the matrices whose  $(i, j)$ -entries are

$$PI_{ij} = \begin{cases} m_i + m_j & \text{if } i \neq j, \text{ and } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & \text{otherwise} \end{cases}$$

and

$$vPI_{ij} = \begin{cases} n_i + n_j & \text{if } i \neq j, \text{ and } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & \text{otherwise} \end{cases}$$

where  $m_i$  and  $n_i$  are, respectively, the number of edges and the number of vertices lying closer to the vertex  $v_i$  than to the vertex  $v_j$ , and where  $m_j$  and  $n_j$  are defined analogously.

For reasons of brevity, the definitions of the **He energy** [26, 12], **second-stage energy** [10], and **common-neighborhood energy** [7] will be skipped.

The eigenvalues of a matrix are the zeros of the respective characteristic polynomial. In particular, the graph eigenvalues are the zeros of the characteristic polynomial of the adjacency matrix. Bearing this in mind, another easily conceivable direction of extending the graph-energy concept is to use the zeros of some graph polynomial and sum their absolute values. Research along these lines could be found in [80, 100]. However, a still more extreme generalization is outlined in the subsequent section.

#### 4. The ultimate energy

Motivated by formula (7), we propose the “ultimate” extension of the energy-concept.

**Definition.** Let  $\mathbf{X} = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n)$  be an arbitrary  $n$ -tuple of real numbers, and let  $\bar{x}$  be their arithmetic mean. Then the *ultimate energy*, associated with  $\mathbf{X}$  is

$$UE = UE(\mathbf{X}) = \sum_{i=1}^n |\mathbf{x}_i - \bar{x}| .$$

We see that  $UE$  is defined without any relation to a graph, to a matrix, or to a polynomial. Yet, even such a parsimonious definition makes it possible to establish some properties of  $UE$ , which then hold for any other energy as well. Emulating McClelland’s approach [82] (which, originally, was stated

for Hückel molecular orbital energy levels) we obtain the following estimates [47]:

$$\sqrt{n \operatorname{Var}(x) + n(n-1) |P(\bar{x})|^{2/n}} \leq UE(\mathbf{X}) \leq n \sqrt{\mathbf{Var}(\mathbf{x})}$$

where  $\operatorname{Var}(x)$  is the variance of the numbers  $x_1, x_2, \dots, x_n$  and  $P(x) = \prod_{i=1}^n (x - x_i)$ . Emulating the considerations from the paper [39], we arrive at an improved upper bound:

$$UE(\mathbf{X}) \leq \sqrt{n(n-1)\mathbf{Var}(\mathbf{x}) + n|\mathbf{P}(\bar{\mathbf{x}})|^{2/n}}.$$

Earlier reported lower and upper bounds for energy, Laplacian energy, distance energy, Randić energy, Harary energy, etc., happen to be special cases of the above bounds for the “ultimate energy”.

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