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Research Article

Relating energy and Sombor energy

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Abstract

It is shown that for every bipartite graph G not containing cycles of size divisible by 4, the graph energy $\mathcal{E}(G)$ and the Sombor energy $\mathcal{E}_{SO}(G)$ are related as $\sqrt{2}\,\delta\,\mathcal{E}(G) \le \mathcal{E}_{SO}(G) \le \sqrt{2}\,\Delta\,\mathcal{E}(G)$, where δ and Δ are the minimum and maximum vertex degrees in G.

Keywords: Sombor index; Sombor energy; energy (of graph); degree (of vertex).

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1. Introduction

Let G be a simple graph with vertex set $\mathbf{V}(G)$ and edge set $\mathbf{E}(G)$, $|\mathbf{V}(G)| = n$, $|\mathbf{E}(G)| = m$. If the vertices $u, v \in \mathbf{V}(G)$ are adjacent, then the edge connecting them is denoted by uv. The number of edges incident to a vertex v is the degree of the vertex v, and is denoted by d_v. The minimum and maximum vertex degrees are denoted by δ and Δ, respectively.

The adjacency matrix $\mathbf{A}(G) = [a_{ij}]$ of the graph G, with vertex set $\mathbf{V}(G) = \{v_1, v_2, \dots, v_n\}$, is the symmetric matrix of order n, whose elements are defined as [3]

$$a_{ij} = \begin{cases} 1 & \text{if } v_i v_j \in \mathbf{E}(G) \\ 0 & \text{if } v_i v_j \notin \mathbf{E}(G) \\ 0 & \text{if } i = j\,. \end{cases} \tag{1}$$

If the eigenvalues of $\mathbf{A}(G)$ are $\lambda_1, \lambda_2, \dots, \lambda_n$, then the (ordinary) *energy* of the graph G is defined as

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

The theory of graph energy is nowadays much studied and is elaborated in full detail [14,19,24].

For other graph-theoretical notions, the readers are referred to textbooks [1,3].

In the chemical and mathematical literature, a great number of vertex-degree-based (VDB) graph invariants of the form

$$TI = TI(G) = \sum_{uv \in \mathbf{E}(G)} \varepsilon(d_u, d_v) \tag{2}$$

have been and are currently considered, where ε is a suitably chosen function, with property $\varepsilon(x,y) = \varepsilon(y,x)$ [16,17,28,29]. Among them is the *Sombor index* [10], for which $\varepsilon(x,y) = \sqrt{x^2 + y^2}$.

In analogy to Equation (1), bearing in mind formula (2), one may introduce the matrix $\mathbf{A}_{TI}(G) = [(a_{TI})_{ij}]$ via

$$(a_{TI})_{ij} = \begin{cases} \varepsilon(d_{v_i}, d_{v_j}) & \text{if } v_i v_j \in \mathbf{E}(G) \\ 0 & \text{if } v_i v_j \notin \mathbf{E}(G) \\ 0 & \text{if } i = j\,. \end{cases} \tag{3}$$

If its eigenvalues are $\lambda_{TI,1}, \lambda_{TI,2}, \dots, \lambda_{TI,n}$, then the "energy" pertaining to the topological index TI, Equation (2), is

$$\mathcal{E}_{TI} = \mathcal{E}_{TI}(G) = \sum_{i=1}^{n} |\lambda_{TI,i}|\,.$$

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For recent works on the investigation of this graph-spectral invariant see [4, 11, 16, 20, 27].

If one chooses $\varepsilon(x,y) = \sqrt{x^2+y^2}$, then, as a special case of the matrix $\mathbf{A}_{TI}$, we get the *Sombor matrix* $\mathbf{A}_{SO}(G)$, whose elements are

$$(a_{SO})_{ij} = \begin{cases} \sqrt{(d_{v_i})^2+(d_{v_j})^2} & \text{if } v_iv_j \in \mathbf{E}(G) \\ 0 & \text{if } v_iv_j \notin \mathbf{E}(G) \\ 0 & \text{if } i=j\,. \end{cases} \tag{4}$$

The sum of the absolute values of the eigenvalues of $\mathbf{A}_{SO}(G)$ is the *Sombor energy*, $\mathcal{E}_{SO} = \mathcal{E}_{SO}(G)$.

The Sombor index SO is a recently invented VDB graph invariant, obtained as a result of geometric considerations [10], that found applications in chemistry [25]. Its mathematical properties are by now studied in much detail (see e.g., [2, 5, 18, 23]). Soon after the introduction of the Sombor index, also the Sombor energy and other spectral properties of the Sombor matrix were examined [7, 8, 12, 15, 21, 32]. Although relations between Sombor index and graph energy were recently studied [30, 31], so far no mathematical connection between graph energy and Sombor energy was established. In the present paper, we provide the first such result, thus contributing towards filling this gap.

We first obtain an auxiliary result.

2. Energy of a weighted bipartite graph

From now on we focus our attention to bipartite graphs. Recall that a graph is bipartite if and only all its cycles (if any) are of even size [1].

Denote by $\phi(G,\lambda)$ the characteristic polynomial of the adjacency matrix $\mathbf{A}(G)$, i.e., $\phi(G,\lambda) = \det\big[\lambda\,\mathbf{I}_n - \mathbf{A}(G)\big]$, where $\mathbf{I}_n$ is the unit matrix of order n [3].

The main result in the spectral theory of bipartite graphs is the formula [3]

$$\phi(G,\lambda) = \lambda^n + \sum_{k\geq 1}(-1)^k\,c(G,k)\,\lambda^{n-2k} \tag{5}$$

where $c(G,k) \geq 0$. The immediate consequence of (5) is that the eigenvalues of G are paired so that $\lambda_i = -\lambda_{n-i+1}$ holds for all $i = 1,2,\ldots,n$ (the "Pairing theorem"). From the Sachs theorem [3, 9, 26] we know that

$$(-1)^k\,c(G,k) = \sum_{\sigma\in\mathcal{S}_{2k}(G)} (-1)^{p(\sigma)}\,2^{c(\sigma)}$$

where $\mathcal{S}_k(G)$ is the set of all Sachs graphs of G possessing exactly $2k$ vertices, and where σ is an element of $\mathcal{S}_{2k}(G)$, containing $p(\sigma)$ components, of which $c(\sigma)$ are cycles.

Let G_w be obtained from the graph G by associating weighs to its edges, so that w_{ij} is the weight of the edge ij. Then in analogy to (5) we have

$$\phi(G_w,\lambda) = \lambda^n + \sum_{k\geq 1}(-1)^k\,c_w(G_w,k)\,\lambda^{n-2k} \tag{6}$$

and by the Sachs theorem

$$(-1)^k\,c_w(G_w,k) = \sum_{\sigma\in\mathcal{S}_{2k}(G_w)} (-1)^{p(\sigma)}\,2^{c(\sigma)}\,w(\sigma)$$

where $w(\sigma)$ is the weight of the Sachs graph σ, equal to the product of the weights of its components. If the isolated edge ij (consisting of two vertices) is a component of σ, then its weight is w_{ij}^2. If a cycle Z is a component of σ, then its weight is the product of weights of its edges [22, 26].

Theorem 2.1. *If the Sachs graph $\sigma \in \mathcal{S}_{2k}(G) \neq \emptyset$ does not contain cycles whose size is divisible by 4, then*

$$(-1)^k\,(-1)^{p(\sigma)}\,2^{c(\sigma)} > 0\,.$$

Proof. The Sachs graph σ has $p(\sigma)$ components. Let among them there are r_0 isolated edges, whose total number of vertices is $2r_0$. Let σ contain r_1 cycles (none of which having size divisible by 4), whose total number of vertices is $4x+2\,r_1$ for some integer x. Thus, $2k = 2r_0 + 4x + 2\,r_1$.

Case 1: k is not divisible by 4. Then $(-1)^k = -1$ whereas $r_0+r_1 = p(\sigma)$ must be odd. Therefore $(-1)^k\,(-1)^{p(\sigma)} > 0$ and the claim of Theorem 2.1 holds.

Case 2: k is divisible by 4. Then $(-1)^k = +1$ whereas $r_0+r_1 = p(\sigma)$ must be even, implying, again, $(-1)^k\,(-1)^{p(\sigma)} > 0$. □

Corollary 2.1. *Let G_w be an edge-weighted bipartite graph whose all cycles (if any) have size not divisible by 4, and let the weights of all its edges be positive-valued. Then for any Sachs graph $\sigma \in \mathcal{S}_{2k}(G_w) \neq \emptyset$, $(-1)^k\,(-1)^{p(\sigma)}\,2^{c(\sigma)} > 0$.*

Corollary 2.2. *The coefficients $c_w(G_w, k)$ in Equation (6), are non-negative and are monotonically increasing functions of the edge-weights.*

Corollary 2.3. *The energy $\mathcal{E}(G_w)$ of the graphs G_w is a monotonically increasing function of the edge-weights.*

3. Main results

The adjacency matrix $\mathbf{A}_{TI}(G)$, Equation (3), could be viewed as the ordinary adjacency matrix of an edge-weighted variant of the graph G. Therefore, if the condition $\varepsilon(d_{v_i}, d_{v_j}) > 0$ holds, and if $\varepsilon(x, y)$ is an increasing function for $x \geq 1$ and $y \geq 1$, then we may apply Corollary 2.3, from which it follows:

Theorem 3.1. *If G is a bipartite graph whose all cycles (if any) have size not divisible by 4, then $\mathcal{E}_{TI}(G)$ is an increasing function of the parameters $\varepsilon(d_{v_i}, d_{v_j})$.*

Let

$$\varepsilon_{min} = \min_{ij \in \mathbf{E}(G)} \varepsilon(d_{v_i}, d_{v_j}) \quad \text{and} \quad \varepsilon_{max} = \max_{ij \in \mathbf{E}(G)} \varepsilon(d_{v_i}, d_{v_j}).$$

Then we have the next result.

Corollary 3.1. *For the graph G satisfying the conditions of Theorem 3.1,*

$$\varepsilon_{min}\,\mathcal{E}(G) \leq \mathcal{E}_{TI} \leq \varepsilon_{max}\,\mathcal{E}(G)\,.$$

Proof. If we replace all elements of $\mathbf{A}_{TI}(G)$, Equation (3), by ε_{min}, then this matrix becomes equal to $\varepsilon_{min}\,\mathbf{A}(G)$, whose energy is $\varepsilon_{min}\,\mathcal{E}(G)$. By Corollary 2.3, this transformation decreases the energy of TI, and we arrive at the left–hand side inequality of Theorem 3.1.

The right–hand side inequality is deduced analogously. □

Theorem 3.2. *If G is a bipartite graph whose all cycles (if any) have size not divisible by 4, then*

$$\sqrt{2}\,\delta\,\mathcal{E}(G) \leq \mathcal{E}_{SO}(G) \leq \sqrt{2}\,\Delta\,\mathcal{E}(G)\,.$$

Proof. Theorem 3.2 is a special case of Corollary 3.1, when it is applied to $\mathbf{A}_{SO}(G)$, Equation (4). Evidently,

$$\sqrt{2}\,\delta \leq \sqrt{(d_{v_i})^2 + (d_{v_j})^2} \leq \sqrt{2}\,\Delta.$$

□

Theorem 3.2 is applicable to trees, in which case $\delta = 1$. It is also applicable to catacondensed hexagonal (benzenoid) systems (= hexagonal systems having no internal vertices) [6,13], which are known to possess only cycles of size not divisible by 4. For these molecular graphs

$$2\sqrt{2}\,\mathcal{E}(G) \leq \mathcal{E}_{SO}(G) \leq 3\sqrt{2}\,\mathcal{E}(G)\,. \tag{7}$$

Hexagonal systems possessing internal vertices, have cycles of size 12 and thus Theorem 3.2 is not applicable. We nevertheless conjecture that the bounds (7) hold to all hexagonal systems.

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