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Research Article

On bond-additive and atoms-pair-additive indices of graphs

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Abstract

For a graph G, its bond-additive indices are defined as $\sum_{uv\in E(G)}\beta(u,v)$, where $E(G)$ is the edge set of G and β is a real-valued function satisfying the property $\beta(u,v)=\beta(v,u)$. By atoms-pair-additive indices of a graph G, we mean graph invariants of the form $\sum_{u,v\in V(G)}\alpha(u,v)/2$, where $V(G)$ is the vertex set of G and α is a real-valued function satisfying $\alpha(u,v)=\alpha(v,u)$. This paper considers some mathematical aspects of several particular bond-additive indices and atoms-pair-additive indices.

Keywords: topological indices; graph invariants; bond-additive indices; atoms-pair-additive indices; chemical graph theory.

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1. Introduction

All graphs considered in this study are assumed to be finite and connected. Let G be such a graph. Its vertex set and edge set are denoted by $V(G)$ and $E(G)$, respectively. In order to avoid trivialities, throughout this paper we assume that $|V(G)|\geq 3$. The edge of G connecting the vertices $u,v\in V(G)$ is denoted by uv. By an n-vertex graph, we mean a graph of order n. The degree and eccentricity of a vertex $v\in V(G)$ are denoted by $d_v(G)$ and $e_u(G)$, respectively. The maximum and minimum degrees of a graph G are denoted by $\Delta(G)$ and $\delta(G)$, respectively. For the vertices $u,v\in V(G)$, the distance between u and v is denoted by $d_G(u,v)$. The transmission $D_G(u)$ of a vertex $u\in V(G)$ is defined by $D_G(u)=\sum_{u\in V(G)}d_G(u,v)$ (see [59, 62]). From the notations $d_v(G)$, $e_u(G)$, $\Delta(G)$, $\delta(G)$, $d_G(u,v)$, $D_G(u)$, we may drop the symbol "G" when there is no confusion about the graph under consideration. We use the standard graph theoretical terminology; notation and terminology used in this paper but not defined here can be found in the books [13, 14, 16, 27].

The degree set of a graph G is the set of all different numbers of the degree sequence of G. A graph G is s-regular if its degree set is $\{s\}$. A graph whose degree set consists of at least two elements is usually referred to as a non-regular graph. By a bidegreed graph, we mean a graph with the degree set having exactly two elements. A semiregular graph G is a bidegreed bipartite graph in which all vertices of each partite set have the same degrees. A graph is said to be strictly stepwise irregular if the difference between the degrees of every pair of adjacent vertices is exactly one; these graphs were recently introduced in [32]. (For every positive integer r, the complete bipartite graph $K_{r,r+1}$ is a strictly stepwise irregular graph.) A self-centered graph (also known as an eccentricity-regular graph) is a connected graph, all of which vertices have the same eccentricity [63]. A transmission-regular graph is the one in which all vertices have the same transmission.

A property of a graph that is opposite to the concept of regularity is known as irregularity; the recent book [4] is fully devoted to the concept of irregularity in graphs. A graph whose all vertices have pair-wise distinct degrees or transmissions is known as an irregular graph or transmission-irregular graph, respectively. Although there is no non-trivial irregular graph [12], there exist transmission-irregular graphs [7]. An n-vertex graph whose degree set consists of $n-1$ elements is known as *antiregular graph* [3, 46, 49].

In graph theory, a graph invariant is a function I defined on the set of all graphs such that the codomain of I contains the extended real numbers and the equation $I(G)=I(G')$ holds if and only if G is isomorphic to G'. A graph invariant may be a matrix (for example, the adjacency matrix), a set of numbers (for example, the spectrum), a polynomial (for example, the characteristic polynomial), a numerical value (for example, order of a graph), etc. In chemical graph theory, numerical graph invariants are usually referred to as topological indices [68]. The first and second Zagreb indices (denoted by M_1 and M_2) (see [23, 30, 35, 64, 65]), Randić index Ra (see [21, 43, 52]), hyper Zagreb index HM (see [22, 24, 61]), sigma index σ

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(see [36, 37]), eccentric-connectivity index ECI (see [17, 45, 51, 60, 69, 72]), Mostar index Mo (see [5, 20, 25, 41]), Albertson index Al (see [2]) are among the most familiar topological indices.

A topological index TI is said to be a graph irregularity index (or irregularity measure) if $TI(G) \geq 0$ and if the equality $TI(G) = 0$ holds if and only if graph G is regular (see [1,2,6,11,31,38,47,54–56]). For a graph G, its topological indices of the form $\sum_{uv \in E(G)} \beta(u,v)$ are known as bond-additive indices [67], where β is a real-valued function satisfying the condition $\beta(u,v) = \beta(v,u)$. By atoms-pair-additive indices of a graph G, we mean topological indices of the form $\sum_{u,v \in V(G)} \alpha(u,v)/2$, where α is a real-valued function with the property $\alpha(u,v) = \alpha(v,u)$. In this study, we are concerned with the mathematical aspects of particular bond-additive indices and atoms-pair-additive indices.

2. Preliminary considerations

An edge uv of an n-vertex graph G is said to be a strong, week, or neutral edge, if $d_u + d_v > n$, $d_u + d_v < n$, or $d_u + d_v = n$, respectively. Based on the definitions of strong, weak, and neutral edges, we define some classes of graphs. A strong graph is the one that contains at least one strong edge and in which every edge is either strong or neutral. We note that regular strong graphs consists of only strong edges. A non-regular strong graph, consisting of only strong edges, is referred to as a non-regular strictly strong graph. A graph containing at least one weak edge, in which every edge is either week or neutral is known as a weak graph. Evidently, regular weak graphs consist of only week edges. A non-regular weak graph consisting of only weak edges is referred to as a non-regular strictly weak graph. A graph having at least one week and at least one strong edge is referred to as a mixed graph. By a neutral graph, we mean a graph consisting of only neutral edges. Examples of non-regular weak and strong graphs are given in Figure 1: T_6, B_6 and D_6 are weak graphs, U_6 is a strictly weak graph, A_5 is a strong graph, and J_6 is a strictly strong graph. Additional examples of regular weak, strong, and neutral graphs are given in Figure 2: G_A, G_B, and G_C are weak graphs, G_D is a strong graph, whereas G_E is a neutral graph.

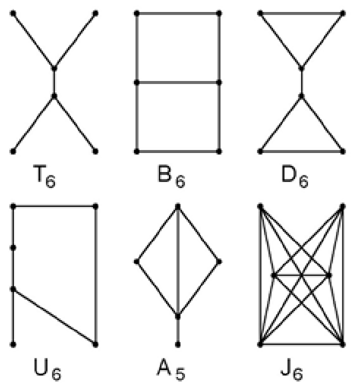

Figure 1: Examples of non-regular weak and strong graphs.

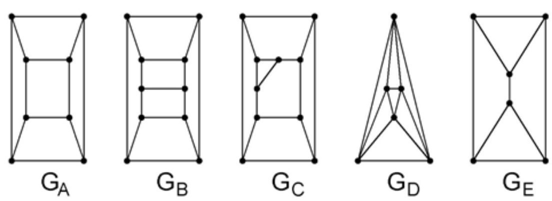

Figure 2: Examples of regular weak, strong and neutral graphs.

Remark 2.1. *It is easy to see that an n-vertex non-regular graph is strictly week if its maximum degree is less than $n/2$. Similarly, an n-vertex non-regular graph is strictly strong if its minimum degree is greater than $n/2$.*

3. On bond-additive indices

Bond-additive indices of a graph G are defined as [67] $\sum_{uv \in E(G)} \beta(u,v)$, where β is a real-valued function satisfying the property $\beta(u,v) = \beta(v,u)$; note that β may take negative values as well. Several examples of bond-additive indices can be found in [10, 15, 50, 53, 57, 58, 66]; most of these can be considered as variants of the first and second Zagreb index (see the review [24]).

The first and second Zagreb indices of a graph G are usually denoted by $M_1(G)$ and $M_2(G)$, and are defined as

$$M_1(G) = \sum_{u \in V(G)} (d_u)^2 = \sum_{uv \in E(G)} (d_u + d_v) \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d_u\, d_v.$$

The Albertson index (introduced under the name "irregularity of a graph" in [2]) is defined as

$$Al(G) = \sum_{uv \in E(G)} |d_u - d_v| \,.$$

Let us consider the following special form of the bond-additive indices

$$BAI(G) = \sum_{uv \in E(G)} W(u,v)\, F(u,v) \tag{1}$$

where W and F are non-negative real-valued symmetric functions. (We remark here that if we drop the condition of non-negativity of W and F in formula (1), then we get an equivalent form of the general bond-additive indices defined in the first sentence of this section.) We call W the weight function. First, we choose the weight function $W(u,v)$ as $d_u + d_v$, $d_u\, d_v$, or $|d_u - d_v|$, and denote the corresponding bond-additive indices in Eq. (1) as $BAI_A(G)$, $BAI_B(G)$, or $BAI_C(G)$, respectively:

$$BAI_A(G) = \sum_{uv \in E(G)} (d_u + d_v)\, F(u,v), \tag{2}$$

$$BAI_B(G) = \sum_{uv \in E(G)} (d_u\, d_v)\, F(u,v), \tag{3}$$

$$BAI_C(G) = \sum_{uv \in E(G)} |d_u - d_v|\, F(u,v). \tag{4}$$

From the above definitions, the next inequalities follow directly for any non-trivial connected graph G:

$$2 \sum_{uv \in E(G)} F(u,v) \le 2\delta \sum_{uv \in E(G)} F(u,v) \le BAI_A(G) \le 2\Delta \sum_{uv \in E(G)} F(u,v) \le 2(n-1) \sum_{uv \in E(G)} F(u,v),$$

$$\sum_{uv \in E(G)} F(u,v) \le \delta^2 \sum_{uv \in E(G)} F(u,v) \le BAI_B(G) \le \Delta^2 \sum_{uv \in E(G)} F(u,v) \le (n-1)^2 \sum_{uv \in E(G)} F(u,v),$$

$$0 \le BAI_C(G) \le (\Delta - \delta) \sum_{uv \in E(G)} F(u,v) \le (n-2) \sum_{uv \in E(G)} F(u,v).$$

From the definition of $BAI_A(G)$, one can deduce various variants of the traditional topological indices. Some particular cases are given as follows:

1. If $F(u,v) = |D_G(u) - D_G(v)|$, then $EMo(G) = \sum_{uv \in E(G)} (d_u + d_v)\, |D_G(u) - D_G(v)|$ is the extended Mostar index (known as additively weighted Mostar index [5]).
2. If $F(u,v) = (d_u - d_v)^2$, then $E\sigma(G) = \sum_{uv \in E(G)} (d_u + d_v)\,(d_u - d_v)^2$ is the extended sigma index of G [36, 37].
3. If $F(u,v) = 1/\sqrt{d_u\, d_v}$, then $ERa(G) = \sum_{uv \in E(G)} (d_u + d_v)\,(d_u\, d_v)^{-1/2}$ is the extended Randić index of G.
4. If $F(u,v) = |d_u - d_v|$, then $EAL(G) = \sum_{uv \in E(G)} (d_u + d_v)\, |d_u - d_v|$ is the extended Albertson index of G.
5. If $F(u,v) = (e_u + e_v)$, then $EECI(G) = \sum_{uv \in E(G)} (d_u + d_v)\,(e_u + e_v)$ is the extended eccentric connectivity index of G.

Similarly, the topological index $BAI_B(G)$ can be regarded as the extended version of the second Zagreb index $M_2(G)$, while the index $BAI_C(G)$ may be considered as the extended version of the Albertson index $Al(G)$. The Mostar index [5, 20] is defined as:

$$Mo(G) = \sum_{uv \in E(G)} |n_u - n_v| \tag{5}$$

where n_u stands for the number of vertices of G closer to u than v, and n_v is defined analogously. Based on the known identity $|D_G(u) - D_G(v)| = |n_u - n_v|$, one obtains that

$$Mo(G) = \sum_{uv \in E(G)} |D_G(u) - D_G(v)| = \sum_{uv \in E(G)} |n_u - n_v|$$

and consequently

$$EMo(G) = \sum_{uv \in E(G)} (d_u + d_v)\, |D_G(u) - D_G(v)| = \sum_{uv \in E(G)} (d_u + d_v)\, |n_u - n_v| \,. \tag{6}$$

Here, it needs to be mentioned that the graph invariant $\sum_{uv \in E(G)} |D_G(u) - D_G(v)|$ was introduced in [59].

4. Some observations

In this section, we report some simple observations and a few results that are used in our upcoming discussion.

Observation 4.1. *Let G be an n-vertex connected graph. Then for any edge uv of G, it holds that*

$$2\delta \le d_u + d_v \le 2\Delta \le 2(n-1).$$

Observation 4.2. *Let G be an n-vertex connected r-regular graph. Then for any edge uv of G, it holds that*

$$d_u + d_v = 2r \le 2(n-1)$$

and equality holds if G is isomorphic to the complete graph K_n.

Remark 4.1. *There exist r-regular neutral graphs different from complete bipartite regular graphs $K_{r,r}$. As an example, see the 6-vertex, 3-regular graph $\mathbf{G}_E$ depicted in Figure 2.*

Proposition 4.1. *A non-regular connected graph G is a neutral graph if and only if G the complete bipartite graph $K_{p,q}$ with $p \neq q$.*

Proof. Since $d_u + d_v = p + q = |V(K_{p,q})|$ for every edge $uv \in E(K_{p,q})$, the complete bipartite graph $K_{p,q}$ is a neutral graph. Conversely, let G be a non-regular connected neutral graph of order n. Then the equation $d_u + d_v = n$ holds for every pair of adjacent vertices $u, v \in V(G)$. Let us consider an arbitrary vertex $w \in V(G)$. Then every neighbor of w has degree $n - d_w$ and every neighbor of all neighbors of w has degree d_w. Thus, the graph G is bidegreed in which adjacent vertices have different degrees; namely d_w and $n - d_w$.

We claim that G is bipartite. Assume to the contrary that G contains an odd cycle, namely $C : v_1v_2 \cdots v_{2r+1}$ where r is a positive integer. Without loss of generality, assume that $d_{v_1} = d_w$ then $d_{v_2} = d_{v_4} = \cdots = d_{v_{2r}} = n - d_w$ and $d_{v_3} = d_{v_5} = \cdots = d_{v_{2r+1}} = d_w$, which gives a contradiction because because v_1 and v_{2r+1} are adjacent. Thus, G contains no odd cycle and hence G is bipartite.

Let (V_1, V_2) be a bipartition of G. It remains to prove that every vertex of V_1 is adjacent to all vertices of V_2. Let $w_1w_2 \in E(G)$ be an arbitrary edge, where $w_1 \in V_1$ and $w_2 \in V_2$. Then $d_{w_1} \le |V_2|$ and $d_{w_2} \le |V_1|$. Thus, the fact that $d_{w_1} + d_{w_2} = n = |V_1| + |V_2|$ implies that w_1 is adjacent to all members of V_2 and w_2 is adjacent to all members of V_1. This completes the proof. □

Lemma 4.1. [14] *Let G be an n-vertex connected triangle-free graph. Then for any edge uv of G, the inequality $d_u + d_v \le n$ holds. Consequently, connected triangle-free graphs (including connected bipartite graphs) are weak graphs.*

Remark 4.2. *It is easy to see that the converse of Lemma 4.1 is not true. There exist graphs containing triangles for which the inequality $d_u + d_v \le n$ is valid. The graph $\mathbf{D}_6$ depicted in Figure 1 contains two triangles, however the inequality $d_u + d_v \le n = 6$ holds for all its edges.*

Lemma 4.2. [22, 72] *Let G be an n-vertex connected graph. Then for any vertex u of G, the inequality $d(u, v) \le e_v \le n - d_v$ holds.*

Observation 4.3. [22, 72] *Let G be an n-vertex connected graph. Then for the vertices u and v of G, the following inequality holds*

$$d_u + d_v \le 2n - (e_u + e_v)$$

where the equality holds for several connected graphs. The smallest graph of such type is the path P_4. It follows that if $e_u + e_v = n$ holds for any edge uv of G, then the above inequality yields $d_u + d_v \le n$.

Observation 4.4. [3, 46, 49] *Two vertices u and v of a connected n-vertex antiregular graph A_n are adjacent if and only if $d_u + d_v \ge n$ holds for any edge uv in G. From this observation it follows that connected antiregular graphs A_n belong to the family of strong graphs. As an example, see the 5-vertex antiregular graph A_5 depicted in Figure 1.*

5. Upper and lower bounds for some bond-additive indices

Proposition 5.1. *If G is either a connected weak graph or a connected triangle-free graph then*

$$BAI_A(G) \le n \sum_{uv \in E(G)} F(u, v). \tag{7}$$

where equality holds if G contains only neutral edges.

Proof. If G is a weak graph then $d_u + d_v \leq n$ for any edge $uv \in E(G)$. Also, if G is triangle-free then from Lemma 4.1, it follows that the inequality $d_u + d_v \leq n$ holds for any edge $uv \in E(G)$. Evidently, equality holds if G contains only neutral edges, i.e., G is a neutral graph. (Such neutral graphs are the complete bipartite graphs $K_{p,q}$.) □

Remark 5.1. *From Proposition 5.1, it follows that the inequality (7) is valid for any bipartite graph (trees, semiregular and strictly stepwise irregular graphs). However, there exist weak graphs containing triangles, for which the inequality (7) is valid; see the graph D_6 in Figure 1.*

Remark 5.2. *Let us define another weighted topological index:*

$$BAI_D(G) = \sum_{uv \in E(G)} \frac{1}{d_u + d_v} F(u, v).$$

For a connected weak graph, the inequality $1/(d_u + d_v) \geq 1/n$ holds for any edge uv in G. This observation gives the following lower bound for a connected weak graph G:

$$BAI_D(G) \geq \frac{1}{n} \sum_{uv \in E(G)} F(u, v)$$

where the equality holds if G is a neutral graph.

Based on Lemma 4.1, we get the following proposition.

Proposition 5.2. *If G is an n-vertex non-regular strictly strong graph then G contains at least one triangle.*

Proposition 5.3. *For every integer $k \geq 3$, there exists at least one $3k$-vertex bidegreed strictly week graph G_k containing exactly k triangles.*

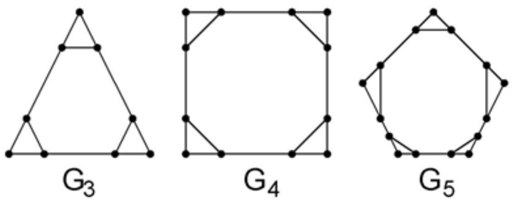

Figure 3: Strictly week graphs G_k having k triangles for $k = 3, 4, 5$.

Proof. The graph G_k containing k triangles is constructed from the cycle C_k, as it is demonstrated in Figure 3. It is easy to check that the inequality

$$\max_{uv \in E(G_k)} (d_u + d_v) = 6 < |V(G_k)|$$

holds.

□

It is easy to show the fulfillment of the following claims.

Proposition 5.4. *Let G_R be an n-vertex R-regular graph.*

(i). If G_R is an R-regular weak graph then

$$BAI_A(G_R) < (2R) \sum_{uv \in E(G_R)} F(u, v).$$

(ii). If G_R is an R-regular strong graph then

$$BAI_A(G_R) > (2R) \sum_{uv \in E(G_R)} F(u, v).$$

(iii). If G_R is an R-regular neutral graph then

$$BAI_A(G_R) = (2R) \sum_{uv \in E(G_R)} F(u, v) = n \sum_{uv \in E(G_R)} F(u, v).$$

Proposition 5.5. *Let A_n be a connected n-vertex antiregular graph. Then*

$$BAI_A(A_n) \geq n \sum_{uv \in E(A_n)} F(u,v). \tag{8}$$

Proof. It is known that connected antiregular graphs are non-regular strong graphs [49]. For them $d_u + d_v \geq n$ holds. □

Observation 5.1. *Let J_n be the graph obtained from the complete graph K_n by removing an edge where $n \geq 4$. The graph J_n is an non-regular strictly strong graph.*

Proof. Observe that $d_u + d_v > n$ for every edge of J_n. □

Proposition 5.6. *For an n-vertex non-regular strictly strong graph G, it holds that*

$$BAI_A(G) > n \sum_{uv \in E(G)} F(u,v). \tag{9}$$

6. Atoms-pair-additive indices

In the previous sections, we restricted our study to the bond-additive indices, defined as the sum of the quantities $\beta(d_u, d_v)$ over all edges (bonds) uv of a (chemical) graph. By extending this concept, we now consider the sum of the quantities $\alpha(u,v)$ over all two-elements sets $\{u,v\}$ of vertices (atoms) of a (chemical) graph, where α is a real-valued function satisfying the condition $\alpha(u,v) = \alpha(v,u)$. (It is possible that α takes negative values as well.) We call these graph invariants atoms-pair-additive indices.

In what follows, we consider the following special type of atoms-pair-additive indices

$$APA(G) = \sum_{\{u,v\} \subseteq V(G)} W(u,v)\, Z(u,v) \tag{10}$$

where $W(u,v)$ and $Z(u,v)$ are appropriately selected non-negative real-valued symmetric functions. Both are defined on the set of the two-elements subsets of $V(G)$.

Many special cases of (10) are known in the literature. The majority of these indices are weighted degree-and-distance-based topological indices. Most of them are considered as the extended versions of the Wiener index $W(G)$; see [1, 8, 9, 18, 19, 26, 28, 29, 33, 34, 39, 40, 42, 44, 48, 54, 70, 71]. Some of the special types of $APA(G)$ are discussed in the following.

Class A. Let $W(u,v) = 1$ and $Z(u,v) = |d_u - d_v|$. Then $APA_A(G) = \frac{1}{2} \sum_{u,v \in V(G)} |d_u - d_v|$. The irregularity index $APA_A(G)$ is known as the total irregularity of G and it was introduced by Abdo et al. in [1].

Class B. If $W(u,v) = Z(u,v) = |d_u - d_v|$, then $APA_B(G) = \frac{1}{2} \sum_{u,v \in V(G)} (d_u - d_v)^2$. This irregularity measure was introduced in [54].

Class C. Let $W(u,v) = d(u,v)$ and $Z(u,v) = d_u + d_v$. Consider the topological index defined as $APA_{C1}(G) = DD(G) = \frac{1}{2} \sum_{u,v \in V(G)} (d_u + d_v)\, d(u,v)$. It is known as the degree-distance index (see [19, 29, 42]).
If $W(u,v) = d(u,v)$ and $Z(u,v) = d_u\, d_v$ then we arrive at the topological index:

$$APA_{C2}(G) = Gut(G) = \frac{1}{2} \sum_{u,v \in V(G)} (d_u\, d_v)\, d(u,v).$$

It is known as the Gutman index [18, 33, 34, 48, 70, 71].
If $W(u,v) = d(u,v)$ and $Z(u,v) = e_u + e_v$ then the corresponding topological index is

$$APA_{C3}(G) = EDS(G) = \frac{1}{2} \sum_{u,v \in V(G)} (e_u + e_v)\, d(u,v)\,.$$

It is called the eccentric-distance-sum index [9, 28, 39, 40, 44].
For $W(u,v) = d(u,v)$ and $Z(u,v) = |e_u - e_v|$, one gets

$$APA_{C4}(G) = EN(G) = \frac{1}{2} \sum_{u,v \in V(G)} |e_u - e_v|\, d(u,v)\,.$$

The topological index $EN(G)$ is known as the extended non-centrality number [70]. It is obvious that $EN(G) = 0$ if and only if G is a self-centered graph.

Class D. If $W(u,v) = 1/d(u,v), u \neq v$, and $Z(u,v) = d_u + d_v$, then one gets

$$APA_{D1}(G) = H_A(G) = \frac{1}{2} \sum_{u,v \in V(G)} \frac{(d_u + d_v)}{d(u,v)},$$

which is known as the additively weighted Harary index [71].
If $W(u,v) = 1/d(u,v), u \neq v$ and $Z(u,v) = d_u\, d_v$, then one gets

$$APA_{D2}(G) = H_M(G) = \frac{1}{2} \sum_{u,v \in V(G)} \frac{d_u\, d_v}{d(u,v)}$$

which is the multiplicatively weighted Harary index [71].

7. Relations between weighted topological indices

In [54], it was proven that

$$APA_B(G) = \frac{1}{2} \sum_{u,v \in V(G)} (d_u - d_v)^2 = n\, M_1(G) - 4\, m^2 = n^2\, Var(G) \tag{11}$$

where $Var(G)$ is the Bell's degree variance of a graph G of order n and size m, defined as [11]

$$Var(G) = \frac{1}{n} \sum_{u \in V(G)} \left(d_u - \frac{2m}{n} \right)^2 = \frac{M_1(G)}{n} - \frac{4m^2}{n^2}.$$

It is easy to show that for a self-centered connected graph G, where $e_u = \varepsilon(G)$ for every vertex $u \in V(G)$, it holds that

$$EDS(G) = \sum_{u \in V(G)} e_u\, D_G(u) = \sum_{u \in V(G)} \varepsilon(G)\, D_G(u) = 2\varepsilon(G)\, W(G).$$

In [40], it was verified that for an n-vertex connected graph G, the inequality $EDS(G) \leq 2(n-\delta)W(G)$ holds, where the equality holds if $G \cong C_4$, G is isomorphic to the 6-vertex 4-regular octahedron graph, or $G \cong K_n$. Recently, the following proposition is proven in [18, 33]: If G is a connected graph of order n, with m edges and p pendent vertices, then

$$DD(G) - Gut(G) \geq W(G) - m + (n-p-2)M_2(G) - \frac{1}{2}(n-p-3)M_1(G) - \frac{1}{2}(2m-n)(2m-n+1)(n-p-1).$$

where $M_1(G)$ and $M_2(G)$ are the first and second Zagreb indices. In the above formula, equality is attained if and only if the distance between any two non-pendent vertices in G is at most 2.

In [59], the following general formula (identity) was presented: If G is a connected graph, then for the topological index $DW(G)$,

$$DW(G) = \frac{1}{2} \sum_{u,v \in V(G)} \big[\omega(u) + \omega(v)\big]\, d(u,v) = \sum_{u \in V(G)} \omega(u)\, D_G(u), \tag{12}$$

where $\omega(u)$ is any quantity associated to (or determined by) the vertex u in G, and $D_G(u)$ is the transmission of the vertex u of G.

Consider now the topological indices $DW_A(G)$ and $DW_B(G)$ defined by

$$DW_A(G) = \frac{1}{2} \sum_{u,v \in V(G)} \big[\omega_A(u) + \omega_A(v)\big]\, d(u,v) = \sum_{u \in V(G)} \omega_A(u)\, D_G(u),$$

$$DW_B(G) = \frac{1}{2} \sum_{u,v \in V(G)} \big[\omega_B(u) + \omega_B(v)\big]\, d(u,v) = \sum_{u \in V(G)} \omega_B(u)\, D_G(u).$$

Then, we have

$$DW_A(G) + DW_B(G) = \sum_{u \in V(G)} \big[\omega_A(u) + \omega_B(u)\big] D_G(u). \tag{13}$$

Based on the above formulas, the following proposition can be obtained.

Proposition 7.1. *If G is an n-vertex graph then*

$$DD(G) + EDS(G) = \sum_{u \in V(G)} (d_u + e_u) D_G(u) \leq n \sum_{u \in V(G)} D_G(u) = 2n\, W(G) \tag{14}$$

where $W(G)$ is the Wiener index of G.

Proof. Note that

$$DD(G) + EDS(G) = \sum_{u \in V(G)} d_u D_G(u) + \sum_{u \in V(G)} e_u D_G(u).$$

Also, by Lemma 4.2, $d_u + e_u \le n$ holds for any vertex u of G. Consequently, one obtains

$$DD(G) + EDS(G) = \sum_{u \in V(G)} (d_u + e_u) D_G(u) \le n \sum_{u \in V(G)} D_G(u) = 2n\, W(G). \tag{15}$$

□

Remark 7.1. *In the above formula, equality hold if $d_u + e_u = n$ for any vertex u of G. There are infinitely many connected graphs for which equality holds in (15). Graphs of such type are the path P_4, cycle C_4, complete graph K_4, the 6-vertex 4-regular octahedron graph, and the infinite sequence of bidegreed graphs $J_n \cong K_n - e$ for $n \ge 4$.*

Consider the so-called transmission distance index $TD(G)$ defined as

$$TD(G) = \frac{1}{2} \sum_{u,v \in V(G)} \big[D_G(u) + D_G(v)\big] d(u,v). \tag{16}$$

Based on Eq. (12), one obtains the following proposition.

Proposition 7.2. *If G is a connected graph then*

$$TD(G) = \sum_{u \in V(G)} D_G(u)^2.$$

From Eq. (16), the following result is obtained.

Proposition 7.3. *Let G be an n-vertex transmission regular graph with $k(G) = D_G(u)$ for any vertex u of G. Then*

$$TD(G) = \frac{1}{2} \sum_{u,v \in V(G)} \big[D_G(u) + D_G(v)\big] d(u,v) = n\, k(G)^2.$$

Proposition 7.4. *If G is a connected graph then*

$$\frac{1}{2} \sum_{u,v \in V(G)} (d_u + d_v)^2\, d(u,v) = \sum_{u \in V(G)} d_u^2\, D_G(u) + 2\, Gut(G). \tag{17}$$

Proof. Using Eq. (12), where $\omega(u) = d_u^2$, one obtains

$$\frac{1}{2} \sum_{u,v \in V(G)} (d_u + d_v)^2\, d(u,v) = \frac{1}{2} \sum_{u,v \in V(G)} \left(d_u^2 + d_v^2\right) d(u,v) + \sum_{u,v \in V(G)} (d_u\, d_v)\, d(u,v)\,.$$

Consequently,

$$\frac{1}{2} \sum_{u,v \in V(G)} (d_u + d_v)^2\, d(u,v) = \sum_{u \in V(G)} d_u^2\, D_G(u) + 2\, Gut(G).$$

□

In an analogous manner, by choosing $\omega(u) = d_u^2$, we obtain the next proposition.

Proposition 7.5. *If G is a connected graph then*

$$\frac{1}{2} \sum_{u,v \in V(G)} (d_u - d_v)^2\, d(u,v) = \sum_{u \in V(G)} d_u^2\, D_G(u) - 2\, Gut(G). \tag{18}$$

Corollary 7.1. *If G is a connected graph then*

$$\frac{1}{2} \sum_{u,v \in V(G)} \left[(d_u + d_v)^2 + (d_u - d_v)^2\right] d(u,v) = 2 \sum_{u \in V(G)} d_u^2\, D_G(u)$$

and

$$\frac{1}{2} \sum_{u,v \in V(G)} \left[(d_u + d_v)^2 - (d_u - d_v)^2\right] d(u,v) = 4\, Gut(G).$$

From Eq. (18) the next corollary follows.

Corollary 7.2. *If G is a connected r-regular graph then*

$$Gut(G) = \sum_{u \in V(G)} d_u^2\, D_G(u) = r^2\, W(G).$$

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