Palestine Journal of Mathematics

Vol.15(3), (2026) , 625–639 © Palestine Polytechnic University-PPU 2026

On a modification of the Schultz index

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Communicated by Kinkar Ch. Das

MSC 2020 Classifications: Primary 05C09, 05C92; Secondary 05C76, 05C25.

Keywords and phrases: topological indices, Schultz index, graph automorphism, graph Cartesian product.

The authors would like to thank the reviewers and editor for their constructive comments and valuable suggestions that improved the quality of our paper

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Abstract. The Schultz index of a graph $\Gamma = (V, E)$ is defined as

$$\mathrm{S}(\Gamma) = \sum_{u \neq v} \big(\deg(u) + \deg(v)\big)\partial(u, v),$$

where $\deg(x)$ denotes the degree of the vertex x, $\partial(x, y)$ the distance between vertices x and y, and the sum runs over all the vertices of Γ. It is known that the automorphism group G of Γ, the set of all permutations of V that preserve adjacencies, describes its symmetry. In this paper, a modification of the Schultz index is proposed, taking into account such symmetry as follows

$$\hat{\mathrm{S}}(\Gamma) = \frac{|V|}{|G|} \sum_{u \in V} \sum_{\sigma \in G} \deg(u)\partial\big(u, \sigma(u)\big),$$

we obtain some of its properties, relations with the Schultz and Graovac-Pisanski indices, as well as expressions involving the orbits induced by the action of G on V, and derive explicit formulae for some known families of graphs and the Cartesian product of two graphs. It is worth mentioning that with this work, the tools available for the topological network analysis are expanded, contributing both to the theoretical understanding of invariants and to their potential use in applied areas where symmetry plays a fundamental role, such as mathematical chemistry or complex network theory.

1 Introduction

Graphs are structures that at first sight seem to be so simple, but when we study them, they turn out to be very interesting and somehow a bit complex. Since their inception, they have been proved to be a useful tool for giving solution to some problems and they have established as an area of mathematics in which a lot of research has been done, giving rise to set up relations with other sciences such as physics, chemistry, biology, and computer science, see [4], [9], and [20]. In graph theory, more specifically in one of its applications to mathematical chemistry, arose the concept of *topological index*, which is a number used to relate the graph of a molecule (a graph where the vertices are atoms and the edges are between two chemically bonded atoms) with some of its physicochemical properties. Among the molecular graphs, the most used in applications of graph theory are those where the hydrogen atoms are disregarded, since their neglect do not cause any ambiguity, these graphs may represent the saturated hydrocarbons, *i.e.*, the molecules of hydrocarbons that contain just single bonds between carbon atoms, for example, the molecular graph of propane can be represented by the path graph P_3.

It is known that there is a large amount of topological indices and most of them have proved to be successful in predicting certain physical, chemical, and pharmacological properties of organic molecules, for example, in 2002, S. Gupta *et al.* [13] investigated the relationship of two graph invariants, the eccentric connectivity and the Wiener indices, about to anti-inflammatory activity,

for a data set consisting of 76 pyrazole carboxylic acid hydrazide analogues; in 2003, E. Estrada [10] used a novel folding degree index, together with other macromolecular descriptors, to study steroid-DB3 antibody interactions; in 2021, Veena M. *et al.* [21] computed the Zagreb and other indices related to eccentricity of molecular graphs of phosphorus containing dendrimers; and in 1989, H. P. Schultz [19] computed the MTI (Molecular Topological Index) for the alkanes and its correlation with the boiling point of them is studied. These indices are defined in terms of some parameters of the graph, such as degrees, distances, and matchings, to name a few. Among these, the Wiener index, proposed in 1947 by H. Wiener [23], was used to study the boiling point of alkanes and it has been investigated from different perspectives to the present day, for example, in 1985 E. R. Canfield *et al.* [5] computed the value of this index for trees; in 2005 A. A. Dobrynin and L. S. Mel'nikov [8] presented infinite families of graphs with increasing cyclomatic number whose Wiener index coincide with that of its line graph; and in 2009 S. G. Wagner *et al.* [22] proved that every sufficiently large integer n is the Wiener index of some caterpillar tree with degree ≤ 3 and the correspondent result for even integers and hexagon type graphs. Another index which emerged in a similar context is the MTI index, introduced in 1989 by H. P. Schultz [19], as mentioned above, who also used it for studying the boiling point of alkanes. In 1994, I. Gutman [14] considered it, and he expressed this index as two summands, disregarding one of them and keeping only the other, naming it the Schultz index, he related it to that of Wiener. Independently, A. A. Dobrynin and A. A. Kochetova [7] defined the same index, calling it the degree distance of a graph, showing some properties of it and comparing it with that of Wiener; in 2022, the authors [2] derived explicit expressions for the Schultz index for some product graphs.

In 1991, A. Graovac and T. Pisanski [12] introduced a modified version of the Wiener index, which later was called the *Graovac-Pisanski index* by M. Ghorbani and S. Klavžar [11]. The main feature of this one is that it considers the symmetry of the graph by taking into account its automorphisms. There are some studies about it, we may mention that in 2015, F. Koorepazan-Moftakhar and A. R. Ashrafi [18] obtained exact values for some fullerenes; A. R. Ashrafi and H. Shabani in 2016 [3] computed the value for the line, subdivision, and total graph of a tree; and in 2017, M. Hakimi-Nezhaad and M. Ghorbani [15] calculated the difference between Wiener and Graovac-Pisanski indices for an infinite family of polyhedral graphs.

Another important and interesting topic in graph theory is that of *graph products*, that, in the same way as in other areas of mathematics, a third structure is constructed from two of them with certain properties. Some examples of graph products are the Cartesian, lexicographic, corona, and tensor, to name a few. Particularly, we are interested in the Cartesian product which has been widely studied, for example, in 1996, S. Klavžar *et al.* [17] obtained a formula for the Szeged index for the Cartesian product; in 2021, Dafik *et al.* [6] obtained the precise value of the resolving strong domination number the cartesian product of graphs; in 2023, the authors [1] computed the clustering coefficient for the Cartesian product, among others, expressing it in terms of the clustering coefficient of the factors.

In this paper, by following the ideas of Graovac and Pisanski, we propose a modified version of the Schultz index considering the automorphisms of the graph, and we give explicit formulas of this index for some graph families and the Cartesian product of two graphs.

2 Preliminaries

In this section, we set some notation and concepts used throughout the paper, which are taken from [16] and [20]. By *graph* we mean a finite, simple graph with no loops and it is denoted by $\Gamma = (V, E)$, where V and E are the *vertices* and *edges* sets, respectively, $|V|$ is called the *order* of Γ and $|E|$ its *size*. For $v \in V$, $\deg(v)$ denotes its *degree*, that is, the number of edges incident to it, if $\deg(v) = k$, for all $v \in V$, we say that Γ is k-*regular*; for $u, v \in V$, a *path* from u to v is a sequence of distinct vertices $u = x_0, x_1, \ldots, x_{r-1}, x_r = v$ such that $x_i x_{i+1} \in E$, for $i = 0, 1, \ldots, r-1$, this sequence is called a $u - v$ *path*; if for any $u, v \in V$ there is a $u - v$ path, Γ is called *connected*; for Γ connected and $u, v \in V$, the *distance* between u and v is

$$\partial(u, v) = \min\{\text{length of } u - v \text{ paths}\},$$

where the length of a $u-v$ path is the number of edges in such a path, and its *diameter* is defined as

$$\operatorname{diam}(\Gamma) = \max\{\partial(u,v) : u, v \in V\}.$$

The *Wiener index* of Γ is defined by the formula

$$\mathrm{W}(\Gamma) = \sum_{u \neq v} \partial(u,v)$$

and the *Schultz index* of Γ as

$$\mathrm{S}(\Gamma) = \frac{1}{2} \sum_{u \in V} \sum_{v \in V} \big(\deg(u) + \deg(v)\big)\partial(u,v).$$

An *automorphism* of Γ is an element $\sigma \in \mathbf{S}_V$ (a permutation of V) which satisfies

$$uv \in E \quad \text{if and only if} \quad \sigma(u)\sigma(v) \in E,$$

the set of automorphisms of Γ is denoted by $\operatorname{Aut}\Gamma$ and it is a subgroup of the symmetric group $\mathbf{S}_V$. In what follows, $\mathbf{S}_n$ denotes the symmetric group on n letters. It is known that if $\sigma \in \operatorname{Aut}\Gamma$, then

- $\deg\big(\sigma(v)\big) = \deg(v)$, for any vertex v;
- $\partial\big(\sigma(u), \sigma(v)\big) = \partial(u,v)$, for all vertices u and v.

As mentioned in the Introduction section, in 1991, Graovac and Pisanski [12] introduced a modification of the Wiener index which considers the symmetry of the graph. This index is called the *Graovac-Pisanski index*, and for a connected graph $\Gamma = (V,E)$ with automorphism group G, it is defined by the expression

$$\hat{\mathrm{W}}(\Gamma) = \frac{|V|}{2|G|} \sum_{v \in V} \sum_{\sigma \in G} \partial(v, \sigma(v)).$$

Now, recall that given a group G and a set X, an *action* of G on X is a map $A : G \times X \to X$ such that

i. $A(1,x) = x$, for all $x \in X$, where $1 \in G$ is the identity;

ii. $A(\sigma\rho, x) = A\big(\sigma, A(\rho,x)\big)$, for all $\sigma, \rho \in G$ and $x \in X$.

The *orbit* of an element $x \in X$ is defined as the set

$$\mathcal{O}(x) = \{A(\sigma,x) : \sigma \in G\},$$

and the collection of all orbits gives a partition of X. The action is called *transitive* if it has exactly one orbit, or equivalently, if for any $x, y \in X$ there exists $\sigma \in G$ such that $A(\sigma,x) = y$. Given $x \in X$, the set of elements of G which fix it is called the *stabilizer* of x and it is a subgroup of G, in symbols,

$$G_x = \{\sigma \in G : A(\sigma,x) = x\}.$$

There is a well-known relation between the order of the orbit of an element and its stabilizer

$$|\mathcal{O}(x)| = (G : G_x),$$

where $(G : G_x)$ denotes the *index* of G_x in G, that is, the number of left cosets of G_x in G, which for finite groups is equal to $|G|/|G_x|$.

Let G be the automorphism group of a graph Γ, it is clear that G acts on V in a natural way as follows

$$A(\sigma, v) = \sigma(v),$$

when this action is transitive, Γ is called a *vertex-transitive graph*.
Let $V_1, \ldots, V_k$ be the orbits induced by this action and consider the stabilizer G_v of a vertex

$v \in V_i$, then $|G_v| = |G|/|V_i|$.
In their paper [12], Graovac and Pisanski showed that the index $\hat{\mathrm{W}}(\Gamma)$ can be expressed in terms of the orbits as

$$\hat{\mathrm{W}}(\Gamma) = |V| \sum_{i=1}^{k} \frac{\mathrm{W}(V_i)}{|V_i|},$$

where $\mathrm{W}(V_i) = \sum_{u \neq v} \partial(u, v)$, and the sum runs over all the elements of V_i.

The following lemmas will be useful for our purposes.

Lemma 2.1. *Let $u, v \in V_i$, then the number of automorphisms sending u to v is precisely $|G_u|$.*

Proof. Consider $\sigma \in G$ such that $\sigma(u) = v$, then for any $\alpha \in G_u$ we have $\sigma\alpha(u) = v$, that is, $\sigma\alpha$ is an automorphism which sends u to v. On the other hand, if γ is an automorphism such that $\gamma(u) = v$, then $\sigma^{-1}\gamma(u) = u$, which implies $\sigma^{-1}\gamma \in G_u$. Hence, $\gamma = \sigma(\sigma^{-1}\gamma)$, that is, any automorphism which sends u to v can be seen as $\sigma\alpha$, with $\alpha \in G_u$. □

Lemma 2.2. *If $u, v \in V_i$ and $w \in V_j$, with i and j not necessarily distinct, then*

$$\sum_{w \in V_j} \partial(u, w) = \sum_{w \in V_j} \partial(v, w).$$

Proof. Let σ be an automorphism which sends u to v, since $\sigma(V_j) = V_j$, for w there exists $x \in V_j$ such that $\sigma(w) = x$, thus, $\partial(u, w) = \partial(v, x)$, so we obtain

$$\sum_{w \in V_j} \partial(u, w) = \sum_{x \in V_j} \partial(v, x).$$

□

Thus, the expression given by Graovac and Pisanski in terms of the orbits

$$\hat{\mathrm{W}}(\Gamma) = |V| \sum_{i=1}^{k} \frac{\mathrm{W}(V_i)}{|V_i|},$$

can be written as follows

$$\hat{\mathrm{W}}(\Gamma) = |V| \sum_{i=1}^{k} \sum_{x \in V_i} \partial(v, x), \tag{2.1}$$

where $v \in V_i$ is any vertex fixed.

3 A modified version of the Schultz index

In this section, a modified version of the Schultz index, which considers the symmetry of a graph, is presented, emulating the Graovac-Pisanski index definition.

Definition 3.1. Let $\Gamma = (V, E)$ be a graph, the *modified Schultz index* of Γ is defined by the formula

$$\hat{\mathrm{S}}(\Gamma) = \frac{|V|}{|G|} \sum_{v \in V} \sum_{\sigma \in G} \deg(v) \partial\big(v, \sigma(v)\big),$$

where G is the automorphism group of Γ.

Observe that for an asymmetric graph (a graph with a trivial automorphism group), the value of this index is zero; thus, the comment above that this index takes into account the symmetry of the graph makes sense.

From now on, any graph we consider is connected, and G will denote its automorphism group, unless we say otherwise.

Example 3.2. Consider the graph Γ shown in Figure 1 and observe that its automorphism group is

$$G = \{1, \sigma_1 = (u\,z)(v\,y), \sigma_2 = (x\,w), \sigma_3 = (u\,z)(v\,y)(x\,w)\},$$

where $(a\,b)$ denotes the transposition that sends a to b and b to a, leaving fixed the other elements. Note that 1 leaves any vertex fixed, so we can omit this automorphism for our computations. Moreover, u, v, y, and z remain fixed under σ_2, and x and w under σ_1. Thus,

$$\begin{aligned}\hat{\mathrm{S}}(\Gamma) &= \frac{|V|}{|G|}\sum_{v\in V}\sum_{\sigma\in G}\deg(v)\partial\big(v,\sigma(v)\big)\\ &= \frac{6}{4}\Big(\deg(u)\big(\partial(u,\sigma_1(u)) + \partial(u,\sigma_3(u))\big)\\ &\quad + \deg(v)\big(\partial(v,\sigma_1(v)) + \partial(v,\sigma_3(v))\big)\\ &\quad + \deg(w)\big(\partial(w,\sigma_2(w)) + \partial(w,\sigma_3(w))\big)\\ &\quad + \deg(x)\big(\partial(x,\sigma_2(x)) + \partial(x,\sigma_3(x))\big)\\ &\quad + \deg(y)\big(\partial(y,\sigma_1(y)) + \partial(y,\sigma_3(y))\big)\\ &\quad + \deg(z)\big(\partial(z,\sigma_1(z)) + \partial(z,\sigma_3(z))\big)\Big),\end{aligned}$$

obtaining $\hat{\mathrm{S}}(\Gamma) = 78$.

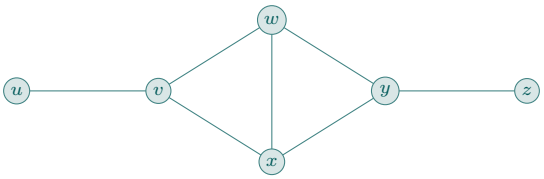


Figure 1. Example of a graph.

Next, we get some results which allow us to relate this index to that of Graovac-Pisanski for regular graphs.

Proposition 3.3. *Let $\Gamma = (V, E)$ be a graph with automorphism group G, if $S \subset V$ is a pointwise fixed set by any $\sigma \in G$ and $\deg(v) = k$, for $v \in V - S$, then*

$$\hat{\mathrm{S}}(\Gamma) = 2k\hat{\mathrm{W}}(\Gamma).$$

Proof. Note that for any $v \in S$ we have $\partial\big(v,\sigma(v)\big) = 0$, thus,

$$\begin{aligned}\hat{\mathrm{S}}(\Gamma) &= \frac{|V|}{|G|}\sum_{v\in V}\sum_{\sigma\in G}\deg(v)\partial\big(v,\sigma(v)\big) = \frac{|V|}{|G|}\sum_{v\in V-S}\sum_{\sigma\in G}\deg(v)\partial\big(v,\sigma(v)\big)\\ &= \frac{|V|}{|G|}\sum_{v\in V-S}\sum_{\sigma\in G}k\partial\big(v,\sigma(v)\big) = k\frac{|V|}{|G|}\sum_{v\in V}\sum_{\sigma\in G}\partial\big(v,\sigma(v)\big).\end{aligned}$$

Hence, $\hat{\mathrm{S}}(\Gamma) = 2k\hat{\mathrm{W}}(\Gamma)$. □

The following corollary follows immediately from the last proposition.

Corollary 3.4. *Let $\Gamma = (V, E)$ be a k-regular graph, then $\hat{\mathrm{S}}(\Gamma) = 2k\hat{\mathrm{W}}(\Gamma)$.*

In what follows, for $U \subset V$ we denote by $\mathrm{S}(U)$ the following expression

$$\mathrm{S}(U) = \frac{1}{2}\sum_{x\in U}\sum_{y\in U}\big(\deg(x) + \deg(y)\big)\partial(x,y), \tag{3.1}$$

where the sum runs over all the elements of U.
Consider the orbits $V_1, \ldots, V_k$ given by the natural action of G over V and observe that Lemma 2.1 ensures that the number of automorphisms sending u to v is precisely $|G_v|$, for any $u, v \in V_i$. Moreover, for $u, v \in V_i$, with u fixed, it is clear that the collection of sets

$$G^{u,v} = \{\sigma \in G : \sigma(u) = v\} = \{\text{automorphisms that send } u \text{ to } v\}$$

gives a partition of G, and the same lemma implies that

$$\begin{aligned}\sum_{\sigma\in G} \partial\big(u,\sigma(u)\big) &= \sum_{v\in V_i}\sum_{\sigma\in G^{u,v}} \partial\big(u,\sigma(u)\big) = \sum_{v\in V_i}\sum_{\sigma\in G^{u,v}} \partial(u,v)\\ &= \sum_{v\in V_i} |G^{u,v}|\partial(u,v) = \sum_{v\in V_i} \frac{|G|}{|V_i|}\partial(u,v).\end{aligned}$$

Since $\deg(u) = \deg(v)$, for $u, v \in V_i$, we may denote by $\deg(V_i)$ the degree of any vertex in V_i, for $i = 1, \ldots, k$.

Theorem 3.5. *Let $\Gamma = (V, E)$ be a graph with automorphism group G, and let $V_1, \ldots, V_k$ be the orbits given by the action of G on V, then*

$$\hat{\mathrm{S}}(\Gamma) = |V| \sum_{i=1}^{k} \frac{\mathrm{S}(V_i)}{|V_i|}.$$

Proof. Observe that since $V = V_1 \cup \cdots \cup V_k$ we get

$$\hat{\mathrm{S}}(\Gamma) = \frac{|V|}{|G|}\sum_{u\in V}\sum_{\sigma\in G} \deg(u)\partial\big(u,\sigma(u)\big) = \frac{|V|}{|G|}\sum_{i=1}^{k}\sum_{u\in V_i}\sum_{\sigma\in G} \deg(u)\partial\big(u,\sigma(u)\big),$$

by the above comments, this expression can be written as follows

$$\begin{aligned}&= \frac{|V|}{|G|}\sum_{i=1}^{k}\left(\sum_{u\in V_i}\sum_{v\in V_i}\frac{|G|}{|V_i|}\deg(V_i)\partial(u,v)\right)\\ &= \frac{|V|}{|G|}\sum_{i=1}^{k}\frac{|G|}{|V_i|}\left(\frac{1}{2}\sum_{u\in V_i}\sum_{v\in V_i} 2\deg(V_i)\partial(u,v)\right)\\ &= \frac{|V|}{|G|}\sum_{i=1}^{k}\frac{|G|}{|V_i|}\left(\frac{1}{2}\sum_{u\in V_i}\sum_{v\in V_i}(\deg(u)+\deg(v))\partial(u,v)\right),\end{aligned}$$

and using Equation 3.1, the above expression can be written as $\frac{|V|}{|G|}\sum_{i=1}^{k}\frac{|G|}{|V_i|}\mathrm{S}(V_i)$. Thus, $\hat{\mathrm{S}}(\Gamma) = |V|\sum_{i=1}^{k}\frac{\mathrm{S}(V_i)}{|V_i|}$. □

Note that this theorem can be taken as an alternative definition for the modified Schultz index of Γ, and an immediate consequence of this is the following result, which relates the Schultz index with the modified one.

Corollary 3.6. *If Γ is a vertex-transitive graph, then $\mathrm{S}(\Gamma) = \hat{\mathrm{S}}(\Gamma)$.*

Next, for a fixed $u \in V_i$ we write $\partial(u, V_i) = \sum_{v\in V_i}\partial(u,v)$, then we have the following.

Corollary 3.7. *The value of $\hat{\mathrm{S}}(\Gamma)$ can be obtained as*

$$\hat{\mathrm{S}}(\Gamma) = |V|\sum_{i=1}^{k}\deg(V_i)\partial(u,V_i),$$

where $u \in V_i$ is fixed.

Proof. Recall that if u, v belong to the same orbit V_i, they have the same degree $\deg(V_i)$. By Proposition 2.2 we have

$$\sum_{w\in V_i} \partial(u,w) = \sum_{w\in V_i} \partial(v,w),$$

for any orbit V_i. Thus,

$$\begin{aligned}
\mathrm{S}(V_i) &= \frac{1}{2}\sum_{u\in V_i}\sum_{v\in V_i}(\deg(u)+\deg(v))\partial(u,v)\\
&= \frac{1}{2}\sum_{u\in V_i}\sum_{v\in V_i} 2\deg(V_i)\partial(u,v) = \deg(V_i)\sum_{u\in V_i}\sum_{v\in V_i}\partial(u,v)\\
&= \deg(V_i)\cdot|V_i|\sum_{v\in V_i}\partial(u,v) = |V_i|\deg(V_i)\partial(u,V_i).
\end{aligned}$$

By the above theorem, we obtain

$$\hat{\mathrm{S}}(\Gamma) = |V|\sum_{i=1}^{k}\frac{\mathrm{S}(V_i)}{|V_i|} = |V|\sum_{i=1}^{k}\frac{|V_i|\deg(V_i)\partial(u,V_i)}{|V_i|}.$$

Hence, $\hat{\mathrm{S}}(\Gamma) = |V|\sum_{i=1}^{k}\deg(V_i)\partial(u,V_i)$. □

The following result gives a tight bound for the value of $\hat{\mathrm{S}}(\Gamma)$.

Proposition 3.8. *Let $\Gamma = (V,E)$ be a graph with orbits $V_1,\dots,V_k$, then*

$$\hat{\mathrm{S}}(\Gamma) \le |V|\operatorname{diam}(\Gamma)\Big(2|E| - \sum_{i=1}^{k}\deg(V_i)\Big).$$

Moreover, this bound is attained by complete graphs.

Proof. For each $i = 1,\dots,k$ consider a fixed vertex $v_i \in V_i$, by the above corollary we have

$$\begin{aligned}
\hat{\mathrm{S}}(\Gamma) &= |V|\sum_{i=1}^{k}\deg(V_i)\partial(v_i,V_i)\\
&\le |V|\sum_{i=1}^{k}\deg(V_i)\operatorname{diam}(\Gamma)(|V_i|-1)\\
&= |V|\operatorname{diam}(\Gamma)\sum_{i=1}^{k}\big(\deg(V_i)|V_i| - \deg(V_i)\big)\\
&= |V|\operatorname{diam}(\Gamma)\Big(\sum_{i=1}^{k}\deg(V_i)|V_i| - \sum_{i=1}^{k}\deg(V_i)\Big),
\end{aligned}$$

but $\sum_{i=1}^{k}\deg(V_i)|V_i| = 2|E|$; thus, $\hat{\mathrm{S}}(\Gamma) \le |V|\operatorname{diam}(\Gamma)\big(2|E| - \sum_{i=1}^{k}\deg(V_i)\big)$.
Now, if K_n denotes the complete graph of order n (defined below, page 634), then it has diameter 1 and size $n(n-1)/2$, its automorphism group is isomorphic to $\mathbf{S}_n$, and V is the only orbit. Thus, the right side of the inequality gives

$$n\big(n(n-1) - (n-1)\big) = n(n-1)^2,$$

which coincides with the expression given below in Proposition 4.4 for complete graphs. □

It is worth mentioning that there is no general relation between the Schultz index and the modified version we are proposing. For example, by using the formula given in [2, Proposition 3.2], for the path graph P_5 (defined below, page 633) we obtain

$$\mathrm{S}(\mathrm{P}_5) = 60,$$

while for the modified one, Proposition 4.1 below gives

$$\hat{S}(P_5) = 40.$$

Thus, $S(P_5) > \hat{S}(P_5)$.
On the other hand, if we consider the complete bipartite graph $K_{2,3}$ (defined below, page 634), we get

$$S(K_{2,3}) = (3+3)2 + 3(2+2)2 + 6(3+2)1 = 66,$$

while for the modified one, Proposition 4.5 below implies

$$\hat{S}(K_{2,3}) = 70.$$

Hence, $S(K_{2,3}) < \hat{S}(K_{2,3})$.

We conclude this section with a table showing the values of the Schultz and the modified Schultz indices, for the graphs associated with the twelve 6-carbon cycloalkane molecules, whose formula is C_6H_{12}, see Figure 2. In this table, it becomes evident that, in general, the more symmetries the graph has, the higher the modified Schultz index value will be.

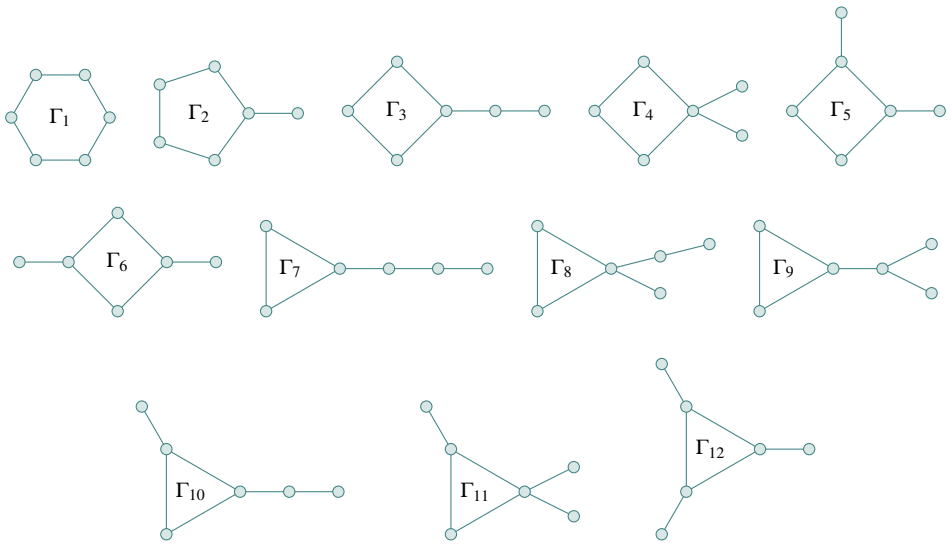


Figure 2. The graphs corresponding to the twelve 6-carbon cycloalkane molecules.

Molecule	Graph	Schultz index	Modified Schultz index
Cyclohexane	Γ_1	108	108
Methylcyclopentane	Γ_2	100	36
Ethylcyclobutane	Γ_3	110	24
1, 1-Dimethylcyclobutane	Γ_4	96	36
1, 2-Dimethylcyclobutane	Γ_5	100	48
1, 3-Dimethylcyclobutane	Γ_6	104	84
Propylcyclopropane	Γ_7	118	12
1-Ethyl-1-methylcyclopropane	Γ_8	98	12
Isopropylcyclopropane	Γ_9	104	24
1-Ethyl-2-methylcyclopropane	Γ_{10}	106	0
1, 1, 2-Trimethylcyclopropane	Γ_{11}	92	12
1, 2, 3-Trimethylcyclopropane	Γ_{12}	96	72

4 The modified Schultz index for some graphs

In this section, we present explicit expressions for the modified Schultz index of some graph families and the Cartesian product of two graphs.

4.1 The modified Schultz index for some graph families

Recall that for any positive integer n, the *path graph* P_n is defined as the graph with vertex set $V = \{v_1, \dots, v_n\}$ and edge set

$$E = \{v_i v_{i+1} : i = 1, \dots, n-1\},$$

it is known that the automorphism group of P_n is isomorphic to $\mathbf{S}_2$, for $n \geq 2$.

Proposition 4.1. *Let n be an integer ≥ 2, then*

$$\hat{\mathrm{S}}(\mathrm{P}_n) = \begin{cases} \frac{n^3-2n^2+2n}{2}, & \textit{for } n \textit{ even}; \\ \frac{n(n-1)^2}{2}, & \textit{otherwise}. \end{cases}$$

Proof. Let 1 and σ be the two automorphisms of P_n, where $\sigma(v_i) = v_{n+1-i}$, for $i = 1, \dots, n$. Thus,

$$\begin{aligned}
\hat{\mathrm{S}}(\mathrm{P}_n) &= \frac{n}{2} \sum_{i=1}^{n} \sum_{\sigma \in S_2} \deg(v_i) \partial\big(v_i, \sigma(v_i)\big) \\
&= \frac{n}{2} \sum_{i=1}^{n} \big(\deg(v_i) \partial\big(v_i, 1(v_i)\big) + \deg(v_i) \partial\big(v_i, \sigma(v_i)\big) \big) \\
&= \frac{n}{2} \sum_{i=1}^{n} \deg(v_i) \partial(v_i, v_{n+1-i}) \\
&= \frac{n}{2} \left(2(n-1) + 2 \sum_{i=2}^{n-1} \partial(v_i, v_{n+1-i}) \right) \\
&= n \left((n-1) + \sum_{i=2}^{n-1} \partial(v_i, v_{n+1-i}) \right).
\end{aligned}$$

If $n = 2k$, we get

$$\begin{aligned}
\hat{\mathrm{S}}(\mathrm{P}_{2k}) &= 2k\big((2k-1) + 2\big((2k-3) + (2k-5) + \cdots + 1\big)\big) \\
&= 2k(2k - 1 + 2(k-1)^2) = 2k(2k^2 - 2k + 1).
\end{aligned}$$

For $n = 2k-1$ note that $\sigma(v_k) = v_k$, hence,

$$\begin{aligned}
\hat{\mathrm{S}}(\mathrm{P}_{2k-1}) &= (2k-1)\big((2k-2) + 2\big((2k-4) + (2k-6) + \cdots + 2\big)\big) \\
&= (2k-1)(2k - 2 + 2(k-2)(k-1)) \\
&= 2(2k-1)(k-1)^2.
\end{aligned}$$

□

For any integer $n \geq 3$, the *cycle graph* C_n is defined as the graph whose vertex set is $V = \{v_1, \dots, v_n\}$ and edge set

$$E = \{v_i v_{i+1} : i = 1, \dots, n\},$$

where $n+1$ is taken as 1. In [2], the authors compute the precise value of $\mathrm{S}(\mathrm{C}_n)$ in Proposition 3.2:

$$\mathrm{S}(\mathrm{C}_n) = \begin{cases} n^3/2, & \text{for } n \text{ even}; \\ (n^3 - n)/2, & \text{otherwise}. \end{cases}$$

Proposition 4.2. *Let n be an integer ≥ 3, then*

$$\hat{\mathrm{S}}(\mathrm{C}_n) = \begin{cases} \frac{n^3}{2}, & \text{for } n \text{ even;} \\ \frac{n^3-n}{2}, & \text{otherwise.} \end{cases}$$

Proof. Since C_n is vertex-transitive, by Corollary 3.6 and the above comment, we have $\hat{\mathrm{S}}(\mathrm{C}_n) = \mathrm{S}(\mathrm{C}_n)$, obtaining the result. □

For any integer $n \geq 3$, the *wheel graph* W_n is defined as the graph with vertex set $V = \{v_0, v_1, \ldots, v_n\}$ and edge set

$$E = \{v_0v_i, v_iv_{i+1} : i = 1, \ldots, n\},$$

where $n+1$ is taken as 1. A well-known fact is that, for $n \geq 4$, the automorphism group of W_n is isomorphic to $\mathbf{D}_n$, the dihedral group of order $2n$.

Proposition 4.3. *Let $n \geq 4$, then $\hat{\mathrm{S}}(\mathrm{W}_n) = 6(n+1)(n-2)$.*

Proof. Observe that $\sigma(v_0) = v_0$, for all $\sigma \in \operatorname{Aut}\mathrm{W}_n$, and $\deg(v_i) = 3$, for $i = 1, \ldots, n$, so we may apply Corollary 3.7, obtaining

$$\hat{\mathrm{S}}(\mathrm{W}_n) = (n+1)(3\partial(v_1, V_1) + n\partial(v_0, V_2)) = 3(n+1)(1+1+2(n-3)).$$

thus, $\hat{\mathrm{S}}(\mathrm{W}_n) = 6(n+1)(n-2)$. □

For any positive integer n, the *complete graph* K_n is the graph of order n where any two distinct vertices are adjacent. In [2] the authors also compute the value of $\mathrm{S}(\mathrm{K}_n)$ in Proposition 3.2, which is

$$\mathrm{S}(\mathrm{K}_n) = n(n-1)^2.$$

Proposition 4.4. *Let n be a positive integer, then $\hat{\mathrm{S}}(\mathrm{K}_n) = n(n-1)^2$.*

Proof. Observe that K_n is a vertex-transitive graph, by Corollary 3.6 and the above comment, we have $\hat{\mathrm{S}}(\mathrm{K}_n) = \mathrm{S}(\mathrm{K}_n) = n(n-1)^2$. □

For any positive integers m and n, the *complete bipartite* graph $\mathrm{K}_{m,n}$ is defined as the graph whose vertex and edge sets are

$$V = \{u_1, \ldots, u_m\} \cup \{v_1, \ldots, v_n\}$$
$$\text{and} \quad E = \{u_iv_j : i = 1, \ldots, m \text{ and } j = 1, \ldots, n\},$$

respectively. It is known that its automorphism group is as follows

$$\operatorname{Aut}\mathrm{K}_{m,n} \cong \begin{cases} \mathbf{S}_m \times \mathbf{S}_n, & \text{if } m \neq n; \\ \mathbf{S}_2[\mathbf{S}_m], & \text{otherwise,} \end{cases}$$

where $\mathbf{S}_2[\mathbf{S}_m]$ denotes the wreath product of $\mathbf{S}_2$ around $\mathbf{S}_m$.

Proposition 4.5. *Let m and n be positive integers, then*

$$\hat{\mathrm{S}}(\mathrm{K}_{m,n}) = \begin{cases} 4mn(m+n) - 2(m+n)^2, & \text{if } n \neq m; \\ 6m^3 - 4m^2, & \text{otherwise.} \end{cases}$$

Proof. Suppose $m \neq n$, then $\operatorname{Aut}\mathrm{K}_{m,n} \cong \mathbf{S}_m \times \mathbf{S}_n$. Consider the partition of the vertex set $V = V_1 \cup V_2$, where V_1 consists of the degree n vertices and V_2 those of degree m. If $u \in V_1$ and $v \in V_2$, by Corollary 3.7 we have

$$\begin{aligned} \hat{\mathrm{S}}(\mathrm{K}_{m,n}) &= |V|\big(\deg(u)\partial(u, V_1) + \deg(v)\partial(v, V_2)\big) \\ &= (m+n)\left(n\sum_{x \in V_1}\partial(u,x) + m\sum_{y \in V_2}\partial(v,y)\right) \\ &= (m+n)\big(2n(m-1) + 2m(n-1)\big) \\ &= (m+n)(4mn - 2m - 2n) \\ &= 4mn(m+n) - 2(m+n)^2. \end{aligned}$$

Now, assume $m = n$, then $\mathrm{K}_{m,m}$ is vertex-transitive, and by Corollary 3.6 we have $\hat{\mathrm{S}}(\mathrm{K}_{m,m}) = \mathrm{S}(\mathrm{K}_{m,m})$. But

$$\begin{aligned}\mathrm{S}(\mathrm{K}_{m,m}) &= \frac{1}{2}\sum_{u\in V}\sum_{v\in V}\big(\deg(u)+\deg(v)\big)\partial(u,v)\\ &= \frac{1}{2}\sum_{u\in V}\sum_{v\in V}2m\partial(u,v) = m\sum_{u\in V}\sum_{v\in V}\partial(u,v)\\ &= m\sum_{u\in V}(3m-2) = m(2m)(3m-2).\end{aligned}$$

Thus, $\hat{\mathrm{S}}(\mathrm{K}_{m,m}) = 6m^3 - 4m^2$. □

For any integer $n \geq 1$, the *star graph* S_n is the graph whose vertex set is $V = \{v_0, v_1, \ldots, v_n\}$ and with edge set

$$E = \{v_0 v_i : i = 1, \ldots, n\}.$$

Observe that S_n can be considered as $\mathrm{K}_{1,n}$, so we have the following.

Corollary 4.6. *Let $n \geq 2$, then $\hat{\mathrm{S}}(\mathrm{S}_n) = 2(n^2-1)$.*

4.2 The modified Schultz index for the Cartesian product of two graphs

In this section, we give the precise value of the modified Schultz index for the Cartesian product of two graphs.

Recall that given two graphs $\Gamma_1 = (V_1, E_1)$ and $\Gamma_2 = (V_2, E_2)$, the *Cartesian product* of Γ_1 and Γ_2 is the graph $\Gamma_1 \times \Gamma_2 = (V, E)$, with $V = V_1 \times V_2$ and

$$E = \{(u,v)(x,y) : u = x \text{ and } vy \in E_2, \text{ or } ux \in E_1 \text{ and } v = y\}.$$

Moreover, if (u,v) and (x,y) are two vertices of $\Gamma_1 \times \Gamma_2$, then

$$\deg(u,v) = \deg(u) + \deg(v) \quad \text{and} \quad \partial\big((u,v),(x,y)\big) = \partial(u,x) + \partial(v,y).$$

A nontrivial graph Γ is called *prime* if it cannot be expressed as the product of two nontrivial graphs. It is known that every nontrivial graph can be expressed as a product of prime graphs. Two graphs Γ_1 and Γ_2 are called *relatively prime*, if there is no nontrivial graph which is a factor of both graphs. For relatively prime graphs Γ_1 and Γ_2 the following relation holds

$$\mathrm{Aut}(\Gamma_1 \times \Gamma_2) \cong \mathrm{Aut}\,\Gamma_1 \times \mathrm{Aut}\,\Gamma_2.$$

Note that, under these conditions, the orbit of the vertex (u,v) is

$$\mathcal{O}(u,v) = \mathcal{O}(u) \times \mathcal{O}(v).$$

In Theorem 4.1 of [2], the authors give the following relation for the Schultz index of the Cartesian product of two graphs,

$$\mathrm{S}(\Gamma_1 \times \Gamma_2) = |V_2|^2\,\mathrm{S}(\Gamma_1) + |V_1|^2\,\mathrm{S}(\Gamma_2) + 4|V_2||E_2|\,\mathrm{W}(\Gamma_1) + 4|V_1||E_1|\,\mathrm{W}(\Gamma_2),$$

using analogous arguments to those in the proof of this theorem, we may show that

$$\begin{aligned}\mathrm{S}(\mathcal{O}(u,v)) =& |\mathcal{O}(u)|^2\,\mathrm{S}(\mathcal{O}(v)) + 2|\mathcal{O}(v)|^2\,\mathrm{W}(\mathcal{O}(u))\deg(\mathcal{O}(v))\\ &+ 2|\mathcal{O}(u)|^2\,\mathrm{W}(\mathcal{O}(v))\deg(\mathcal{O}(u)) + |\mathcal{O}(v)|^2\,\mathrm{S}(\mathcal{O}(u)).\end{aligned}$$

Theorem 4.7. *Let $\Gamma_1 = (V, E_1)$ and $\Gamma_2 = (U, E_2)$ be two relatively prime graphs, with $V = \{v_1, \ldots, v_n\}$ and $U = \{u_1, \ldots, u_m\}$, then*

$$\hat{\mathrm{S}}(\Gamma_1 \times \Gamma_2) = |V|^2\hat{\mathrm{S}}(\Gamma_2) + |U|^2\hat{\mathrm{S}}(\Gamma_1) + 4|V||E_1|\hat{\mathrm{W}}(\Gamma_2) + 4|U||E_2|\hat{\mathrm{W}}(\Gamma_1).$$

Proof. Let $G_1 = \operatorname{Aut}\Gamma_1$ and $G_2 = \operatorname{Aut}\Gamma_2$, since Γ_1 and Γ_2 are relatively prime, we have $\operatorname{Aut}(\Gamma_1 \times \Gamma_2) \cong G_1 \times G_2$. Consider the orbits $V_1, ..., V_k$ and $U_1, ..., U_l$ of the action of G_1 on V_1 and of G_2 on V_2, respectively. By Theorem 3.5, we have

$$\hat{\mathrm{S}}(\Gamma_1 \times \Gamma_2) = |V||U| \sum_{i=1}^{k} \sum_{j=1}^{l} \frac{\mathrm{S}(V_i \times U_j)}{|V_i||U_j|},$$

and by the above comment, we obtain that this expression is equal to the following

$$\begin{aligned}
&= |V||U| \sum_{i=1}^{k} \sum_{j=1}^{l} \frac{1}{|V_i||U_j|} \big(|U_j|^2\, \mathrm{S}(V_i) + 2|V_i|^2\, \mathrm{W}(U_j) \deg(V_i) \\
&\quad + 2|U_j|^2\, \mathrm{W}(V_i) \deg(U_j) + |V_i|^2\, \mathrm{S}(U_j)\big) \\
&= |V||U| \sum_{j=1}^{l} |U_j| \sum_{i=1}^{k} \frac{\mathrm{S}(V_i)}{|V_i|} + 2|V||U| \sum_{i=1}^{k} |V_i| \deg(V_i) \sum_{j=1}^{l} \frac{\mathrm{W}(U_j)}{|U_j|} \\
&\quad + 2|V||U| \sum_{j=1}^{l} |U_j| \deg(U_j) \sum_{i=1}^{k} \frac{\mathrm{W}(V_i)}{|V_i|} + |V||U| \sum_{i=1}^{k} |V_i| \sum_{j=1}^{l} \frac{\mathrm{S}(U_j)}{|U_j|} \\
&= |U|^2 \hat{\mathrm{S}}(\Gamma_1) + 2|V| \sum_{i=1}^{k} |V_i| \deg(V_i) \hat{\mathrm{W}}(\Gamma_2) \\
&\quad + 2|U| \sum_{j=1}^{l} |U_j| \deg(U_j) \hat{\mathrm{W}}(\Gamma_1) + |V|^2 \hat{\mathrm{S}}(\Gamma_2).
\end{aligned}$$

Since

$$\sum_{i=1}^{k} |V_i| \deg(V_i) = 2|E_1| \quad \text{and} \quad \sum_{j=1}^{l} |U_i| \deg(U_i) = 2|E_2|,$$

the result follows. □

Unlike the previous situation, if we consider a graph Γ, with automorphism group G, then the automorphism group of the Cartesian product of Γ with itself satisfies

$$\operatorname{Aut}(\Gamma \times \Gamma) \cong \mathbf{S}_2[G].$$

Furthermore, it is not difficult to prove that the orbit of a vertex (u, v) is given by

$$\mathcal{O}(u, v) = \big(\mathcal{O}(u) \times \mathcal{O}(v)\big) \cup \big(\mathcal{O}(v) \times \mathcal{O}(u)\big).$$

Observe that $\mathcal{O}(u, v) = \mathcal{O}(v, u)$.

Theorem 4.8. *Let $\Gamma = (V, E)$ be a graph, then*

$$\hat{\mathrm{S}}(\Gamma \times \Gamma) = |V|^2 \hat{\mathrm{S}}(\Gamma) + 4|V||E| \hat{\mathrm{W}}(\Gamma) + 2|V|^2\, \mathrm{S}(\Gamma).$$

Proof. Let G be the automorphism group of Γ and let $V_1, \ldots, V_k$ be the orbits induced by the action of G on V. Consider the orbits induced by the action of $\mathbf{S}_2[G]$ on $V \times V$,

$$V_{ij} = \big(V_i \times V_j\big) \cup \big(V_j \times V_i\big), \quad \text{for } i = 1, \ldots, k \text{ and } j \geq i.$$

Since $V_{ij} = V_{ji}$, for any $a = (u, v) \in V_{ij}$, with $i \neq j$, we get

$$\begin{aligned}
\partial(a, V_{ij}) &= \sum_{b \in V_{ij}} \partial(a, b) = \sum_{(x,y) \in V_i \times V_j} \big(\partial((u, v), (x, y)) + \partial((u, v), (y, x))\big) \\
&= \sum_{x \in V_i} \sum_{y \in V_j} \big(\partial(u, x) + \partial(v, y) + \partial(u, y) + \partial(v, x)\big),
\end{aligned}$$

and for $i = j$, we obtain

$$\partial(a, V_{ii}) = \frac{1}{2} \sum_{x \in V_i} \sum_{y \in V_i} \big(\partial(u,x) + \partial(v,y) + \partial(u,y) + \partial(v,x)\big).$$

Thus, by Corollary 3.7, for $a_{ij} = (u_i, v_j) \in V_{ij}$ we have

$$\hat{\mathrm{S}}(\Gamma \times \Gamma) = |V|^2 \bigg(\frac{1}{2} \sum_{i=1}^{k} \sum_{j \neq i} \deg(a_{ij}) \partial(a_{ij}, V_{ij}) + \sum_{i=1}^{k} \deg(a_{ii}) \partial(a_{ii}, V_{ii}) \bigg),$$

by the above comments, the last expression can be expressed as follows

$$= |V|^2 \bigg(\frac{1}{2} \sum_{i=1}^{k} \sum_{j \neq i} \deg(u_i, v_j) \sum_{x \in V_i} \sum_{y \in V_j} \big(\partial(u_i, x) + \partial(v_j, y) + \partial(u_i, y) + \partial(v_j, x)\big)$$

$$+ \sum_{i=1}^{k} \deg(u_i, v_i) \frac{1}{2} \sum_{x \in V_i} \sum_{y \in V_i} \big(\partial(u_i, x) + \partial(v_i, y) + \partial(u_i, y) + \partial(v_i, x)\big) \bigg),$$

since $\deg(u_i, v_j) = \deg(u_i) + \deg(v_j)$, $\deg(u_i) = \deg(V_i)$, and $\deg(v_j) = \deg(V_j)$, we get

$$= \frac{1}{2} |V|^2 \bigg(\sum_{i=1}^{k} \sum_{j=1}^{k} \big(\deg(V_i) + \deg(V_j)\big) \sum_{x \in V_i} \sum_{y \in V_j} \big(\partial(u_i, x) + \partial(v_j, y)$$

$$+ \partial(u_i, y) + \partial(v_j, x)\big) \bigg)$$

$$= \frac{1}{2} |V|^2 \bigg(\sum_{i=1}^{k} \sum_{j=1}^{k} \big(\deg(V_i) + \deg(V_j)\big) \Big(|V_j| \sum_{x \in V_i} \partial(u_i, x) + |V_i| \sum_{y \in V_j} \partial(v_j, y)$$

$$+ |V_i| \sum_{y \in V_j} \partial(u_i, y) + |V_j| \sum_{x \in V_i} \partial(v_j, x) \Big) \bigg)$$

$$= \frac{1}{2} |V|^2 \bigg(\sum_{i=1}^{k} \sum_{j=1}^{k} \deg(V_i) |V_j| \sum_{x \in V_i} \partial(u_i, x) + \sum_{i=1}^{k} \sum_{j=1}^{k} \deg(V_j) |V_j| \sum_{x \in V_i} \partial(u_i, x)$$

$$+ \sum_{i=1}^{k} \sum_{j=1}^{k} \deg(V_i) |V_i| \sum_{y \in V_j} \partial(v_j, y) + \sum_{i=1}^{k} \sum_{j=1}^{k} \deg(V_j) |V_i| \sum_{y \in V_j} \partial(v_j, y)$$

$$+ \sum_{i=1}^{k} \sum_{j=1}^{k} \big(\deg(V_i) + \deg(V_j)\big) |V_i| \sum_{y \in V_j} \partial(u_i, y)$$

$$+ \sum_{i=1}^{k} \sum_{j=1}^{k} \big(\deg(V_i) + \deg(V_j)\big) |V_j| \sum_{x \in V_i} \partial(v_j, x) \bigg),$$

now, since $\partial(V_i, V_j) = \sum_{x \in V_i} \sum_{y \in V_j} \partial(x, y)$ and Lemma 2.2, we obtain

$$= \frac{1}{2} |V|^2 \bigg(\sum_{i=1}^{k} \deg(V_i) \sum_{x \in V_i} \partial(u_i, x) \sum_{j=1}^{k} |V_j| + \sum_{i=1}^{k} \sum_{x \in V_i} \partial(u_i, x) \sum_{j=i}^{k} \deg(V_j) |V_j|$$

$$+ \sum_{i=1}^{k} \deg(V_i) |V_i| \sum_{j=1}^{k} \sum_{y \in V_j} \partial(v_j, y) + \sum_{i=1}^{k} |V_i| \sum_{j=1}^{k} \deg(V_j) \sum_{y \in V_j} \partial(v_j, y)$$

$$+ \sum_{i=1}^{k} \sum_{j=1}^{k} \big(\deg(V_i) + \deg(V_j)\big) \partial(V_i, V_j)$$

$$+ \sum_{i=1}^{k} \sum_{j=1}^{k} \big(\deg(V_i) + \deg(V_j)\big) \partial(V_j, V_i) \bigg),$$

next, using $\sum_{i=1}^{k}|V_i| = |V|$ and $\sum_{i=1}^{k}\deg(V_i)|V_i| = 2|E|$, we have

$$= \frac{1}{2}|V|^2\Bigg(\sum_{i=1}^{k}\deg(V_i)\partial(u_i,V_i)|V| + 2|E|\sum_{i=1}^{k}\partial(u_i,V_i)$$
$$+ 2|E|\sum_{j=1}^{k}\partial(v_j,V_j) + |V|\sum_{j=1}^{k}\deg(V_j)\partial(v_j,V_j) + 4\,\mathrm{S}(\Gamma)\Bigg),$$

finally, by Corollary 3.7 and Equation 2.1, the last expression is expressed as

$$= \frac{1}{2}|V|^2\left(2\hat{\mathrm{S}}(\Gamma) + 8|E|\frac{\hat{\mathrm{W}}(\Gamma)}{|V|} + 4\,\mathrm{S}(\Gamma)\right).$$

Hence, $\hat{\mathrm{S}}(\Gamma\times\Gamma) = |V|^2\hat{\mathrm{S}}(\Gamma) + 4|E||V|\hat{\mathrm{W}}(\Gamma) + 2|V|^2\,\mathrm{S}(\Gamma)$. □

For the following result, we need to make the following comment. In the paper [12], the expression given for the Graovac-Pisanski index of paths has an inaccuracy; it says

$$\hat{\mathrm{W}}(\mathrm{P}_n) = \begin{cases} \frac{n^3}{2}, & \text{for } n \text{ even;} \\ \frac{n(n^2-1)}{2}, & \text{otherwise} \end{cases}$$

and it should read

$$\hat{\mathrm{W}}(\mathrm{P}_n) = \begin{cases} \frac{n^3}{8} & \text{for } n \text{ even;} \\ \frac{n(n^2-1)}{8} & \text{otherwise.} \end{cases}$$

Recall that for any positive integers m and n, the *grid graph* $\mathrm{G}_{m,n}$ is defined as the Cartesian product of the path graphs P_m and P_n.

Corollary 4.9. *Let m and n be two positive integers, then the modified Schultz index of $\mathrm{G}_{m,n}$ is given by one of the following expressions.*

• *For m and n even,*

$$\hat{\mathrm{S}}(\mathrm{G}_{m,n}) = \begin{cases} \frac{mn}{2}\big((m+n)(2-m-n) + 2mn(m+n-1)\big), & \text{if } m \neq n; \\ \frac{m^3}{6}(14m^2 - 21m + 10), & \text{otherwise.} \end{cases}$$

• *For m and n odd,*

$$\hat{\mathrm{S}}(\mathrm{G}_{m,n}) = \begin{cases} \frac{mn}{2}\big(2 - (m+n)^2 + 2mn(-1+m+n)\big), & \text{if } m \neq n \\ \frac{m^2}{6}(14m^3 - 21m^2 + 4m + 3), & \text{otherwise.} \end{cases}$$

• *For m even and n odd,*

$$\hat{\mathrm{S}}(\mathrm{G}_{m,n}) = \frac{mn}{2}\big(1 - m^2 + n(2-n) + 2mn(m+n-2)\big).$$

Proof. We proceed by cases. Suppose m and n are both even and $m \neq n$, Theorem 4.7 and Proposition 4.1 imply

$$\hat{\mathrm{S}}(\mathrm{G}_{m,n}) = m^2\hat{\mathrm{S}}(\mathrm{P}_n) + n^2\hat{\mathrm{S}}(\mathrm{P}_m) + 4m(m-1)\hat{\mathrm{W}}(\mathrm{P}_n) + 4n(n-1)\hat{\mathrm{W}}(\mathrm{P}_m)$$
$$= m^2\left(\frac{n^3 - 2n^2 + 2n}{2}\right) + n^2\left(\frac{m^3 - 2m^2 + 2m}{2}\right)$$
$$+ 4m(m-1)\left(\frac{n^3}{8}\right) + 4n(n-1)\left(\frac{m^3}{8}\right),$$

obtaining $\hat{\mathrm{S}}(\mathrm{G}_{m,n}) = \frac{mn}{2}\big((m+n)(2-m-n) + 2mn(m+n-1)\big)$.
Now, if $m = n$ and m is even, by Theorem 4.8, Proposition 4.1, and [2, Proposition 3.2] we have

$$\hat{\mathrm{S}}(\mathrm{G}_{m,m}) = m^2\hat{\mathrm{S}}(\mathrm{P}_m) + 4m(m-1)\hat{\mathrm{W}}(\mathrm{P}_m) + 2m^2\,\mathrm{S}(\mathrm{P}_m)$$
$$= m^2\left(\frac{n^3 - 2n^2 + 2n}{2}\right) + 4m(m-1)\left(\frac{m^3}{8}\right)$$
$$+ 2m^2\left(\frac{m(m-1)(2m-1)}{3}\right),$$

so we get $\hat{\mathrm{S}}(\mathrm{G}_{m,m}) = \frac{m^3}{6}(14m^2 - 21m + 10)$.
The other expressions are obtained by analogous procedures. □

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Received: 2025-10-03
Accepted: 2026-01-05