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The modified Schultz index of graph operations

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ABSTRACT. Given a simple and connected graph G with vertex set V, denoting by $d_G(u)$ the degree of a vertex u and $d_G(u,v)$ the distance of two vertices, the modified Schultz index of G is given by $S^*(G) = \sum_{\{u,v\}\subseteq V} d_G(u)\, d_G(v)\, d_G(u,v)$, where the summation goes over all non ordered pairs of vertices of G. In this paper we consider some graph operations, namely cartesian product, complete product, composition and subdivision, and we obtain explicit formulae for the modified Schultz index of a graph in terms of the number of vertices and edges as well as some other topological invariants such as the Wiener index, the Schultz index and the first and second Zagreb indices.

1. INTRODUCTION

Let $G = (V,E)$ be a simple and connected graph. The cardinality of V is called the order and the cardinality of E is called the dimension of G . The elements of E are denoted by uv, where u and v are the end-vertices of the edge uv. For a vertex $u \in V$, $d_G(u)$ denotes the degree of u and the distance between two vertices u and v is $d_G(u,v)$, the length of the shortest path between vertices u and v. The distance from a vertex w to an edge $e = u_1u_2$ is $d^*_G(w,e) = \min\{d_G(w,u_1), d_G(w,u_2)\}$ and the distance between two edges e and f is $D_G(e,f) = \min\{d^*_G(u_1,f), d^*_G(u_2,f)\}$.

The *Wiener index* of G, introduced by H. Wiener in 1947 [12] and defined by $W(G) = \sum_{\{u,v\}\subseteq V} d_G(u,v)$, is widely studied in the literature. The *edge Wiener index* is defined by $W_e(G) = \sum_{\{f,g\}\subseteq E} D_G(f,g)$ [7].

The line graph $L(G)$ of a nonempty graph G is the graph whose vertex set can be put in one-to-one correspondence with the edge set of G in such a way that two vertices of $L(G)$ are adjacent if and only if the corresponding edges of G are adjacent. Since $D_G(f,g) = d_{L(G)}(f,g) - 1$, for all $f,g \in E$, an immediate consequence [8] is that

$$W(L(G)) = W_e(G) + \binom{|E|}{2}. \tag{1.1}$$

The *Schultz index* of G, $S(G) = \sum_{\{u,v\}\subseteq V} (d_G(u) + d_G(v))\, d_G(u,v)$, often called *the degree distance of a graph* (see [3], [4], [6], [11] for more references) has been shown to be a useful graph theoretical descriptor in the design of molecules with desired properties namely to characterize alkalenes by an integer number. Schultz index and the Wiener index are closely related quantities for trees ([5], [10]). Other indices that can be seen as molecular structure-descriptors are the first and second Zagreb indices. The *first Zagreb index* is equal to the sum of squares of the degrees of all vertices, $Z_1(G) = \sum_{u\in V} d^2_G(u) = \sum_{uv\in E} d_G(u) + d_G(v)$, and the *second Zagreb index* is $Z_2(G) = \sum_{uv\in E} d_G(u)d_G(v)$. Analogously, the *first Zagreb coindex* is $\overline{Z}_1(G) = \sum_{uv\notin E}(d_G(u) + d_G(v))$ and the *second Zagreb coindex* is given by $\overline{Z}_2(G) = \sum_{uv\notin E} d_G(u)d_G(v)$.

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The *modified Schultz index* of G, also known (see [1]) as *Schultz index of the second kind* and even also as *Gutman index*, is defined by

$$S^*(G) = \sum_{\{u,v\}\subseteq V} d_G(u)\, d_G(v)\, d_G(u,v),$$

where the summation goes over all non ordered pairs of vertices of G. For a graph $G = (V,E)$ and $V' \subseteq \{\{u,v\} : u,v \in V\}$, we set $S^*_{V'}(G) = \sum_{\{u,v\}\in V'} d_G(u) d_G(v) d_G(u,v)$.

In this paper we give explicit formulas for the modified Schultz index of simple connected graphs, under several operations in terms of its order and dimension and other known graph invariants, such as the Wiener index, the Schultz index and Zagreb indices.

2. Main results

The aim of this section is to compute the modified Schultz index for some graph operations, namely complete product (also known as join), cartesian product, composition and subdivision. We start with a lemma that is widely used in the rest of the paper.

Lemma 2.1. [2] *If $G = (V,E)$ is a graph of order n and dimension q then*

(a) $\overline{Z}_1(G) = 2\,q\,(n-1) - Z_1(G)$.
(b) $\overline{Z}_2(G) = 2\,q^2 - \frac{1}{2} Z_1(G) - Z_2(G)$.

2.1. **Complete product.** The *complete product* $G = G_1 \nabla G_2$ of graphs G_1 and G_2 with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2 is the graph union $G_1 \cup G_2$ together with all edges joining each vertex of V_1 to each vertex of V_2.

Lemma 2.2. [9]*Let G_i be a connected graph of order n_i and dimension q_i, $i = 1,2$. Then*

(a) $$Z_1(G_1 \nabla G_2) = \sum_{\substack{i,j=1\\ i\neq j}}^{2} \big(Z_1(G_i) + 4q_i n_j + n_i n_j^2\big).$$

(b) $$Z_2(G_1 \nabla G_2) = \sum_{\substack{i,j=1\\ i\neq j}}^{2} \Big(n_i Z_1(G_j) + Z_2(G_i) + 2q_i q_j + 2n_i n_j q_i + n_i^2 q_j + \frac{1}{2} n_i^2 n_j^2\Big).$$

Theorem 2.1. *Let $G_i = (V_i, E_i)$ be a connected graph of order n_i and dimension q_i, for $i = 1,2$ and $G = G_1 \nabla G_2$. Then the modified Schultz index of G is*

(a) $$S^*(G) = \sum_{\substack{i,j=1\\ i\neq j}}^{2} \Big((2q_i + n_i n_j)^2 - n_i q_j (n_i + 4) + 2q_i q_j - n_i^2 n_j + n_i n_j\, q - \tfrac{1}{2} n_i^2 n_j^2 - (n_i+1) Z_1(G_j) - Z_2(G_i)\Big)$$

(b) $S^*(G) = 4\,q^2 - (Z_1(G) + Z_2(G))$, *where* $q = |E(G)| = q_1 + q_2 + n_1\, n_2$.

Proof. Notice that $d_G(u) = d_{G_1}(u) + n_2$ if $u \in V_1$ and $d_G(v) = d_{G_2}(v) + n_1$ if $v \in V_2$. Furthermore,

$$d_G(u,v) = \begin{cases} 0 & \text{if } u = v \\ 1 & \text{if } uv \in E_1 \text{ or } uv \in E_2 \text{ or } (u \in V_1 \text{ and } v \in V_2) \\ 2 & \text{otherwise.} \end{cases}$$

Hence, the modified Schultz index of G is given by

$$S^*(G) = S^*_{V_{11}}(G) + S^*_{V_{22}}(G) + S^*_{V_{12}}(G), \tag{2.2}$$

where $V_{ij} = \{\{u,v\} : u \in V_i,\ v \in V_j\}$, $1 \le i \le j \le 2$.

Using Lemma 2.1, we obtain

$$
\begin{aligned}
S^*_{V_{11}}(G) &= \sum_{uv\in E_1} d_G(u)d_G(v)d_G(u,v) + \sum_{\substack{\{u,v\}\subseteq V_1\\ uv\notin E_1}} d_G(u)d_G(v)d_G(u,v)\\
&= \sum_{uv\in E_1} (d_{G_1}(u)+n_2)(d_{G_1}(v)+n_2) + 2\sum_{\substack{\{u,v\}\subseteq V_1\\ uv\notin E_1}} (d_{G_1}(u)+n_2)(d_{G_1}(v)+n_2)\\
&= \sum_{\{u,v\}\subseteq V_1} (d_{G_1}(u)+n_2)(d_{G_1}(v)+n_2) + \sum_{\substack{\{u,v\}\subseteq V_1\\ uv\notin E_1}} (d_{G_1}(u)+n_2)(d_{G_1}(v)+n_2)\\
&= \sum_{\{u,v\}\subseteq V_1} d_{G_1}(u)d_{G_1}(v) + n_2\sum_{\{u,v\}\subseteq V_1} (d_{G_1}(u)+d_{G_1}(v)) + \sum_{\{u,v\}\subseteq V_1} n_2^2\\
&\quad + \sum_{\substack{\{u,v\}\subseteq V_1\\ uv\notin E_1}} d_{G_1}(u)d_{G_1}(v) + n_2\sum_{\substack{\{u,v\}\subseteq V_1\\ uv\notin E_1}} (d_{G_1}(u)+d_{G_1}(v)) + \sum_{\substack{\{u,v\}\subseteq V_1\\ uv\notin E_1}} n_2^2\\
&= 2\overline{Z_2}(G_1) + Z_2(G_1) + n_2\Big(2\overline{Z_1}(G_1) + Z_1(G_1)\Big) + n_2^2\Big(2\binom{n_1}{2} - q_1\Big)\\
&= 4q_1^2 + 4q_1n_2(n_1-1) + (n_1n_2)^2 - n_2^2(n_1+q_1) - (1+n_2)Z_1(G_1) - Z_2(G_1). \qquad (2.3)
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
S^*_{V_{22}}(G) &= 4q_2^2 + 4q_2n_1(n_2-1) + (n_1n_2)^2 - n_1^2(n_2+q_2)\\
&\quad -(1+n_1)Z_1(G_2) - Z_2(G_2). \qquad (2.4)
\end{aligned}
$$

Finally, the last term in (2.2) is:

$$
\begin{aligned}
S^*_{V_{12}}(G) &= \sum_{\{u,v\}\in V_{12}} (d_{G_1}(u)+n_2)(d_{G_2}(v)+n_1)\\
&= \sum_{\{u,v\}\in V_{12}} (d_{G_1}(u)d_{G_2}(v) + n_1d_{G_1}(u) + n_2d_{G_2}(v) + n_1n_2)\\
&= \sum_{\{u,v\}\in V_{12}} d_{G_1}(u)d_{G_2}(v) + n_1n_2\sum_{u\in V_1} d_{G_1}(u) + n_1n_2\sum_{v\in V_2} d_{G_2}(v) + (n_1n_2)^2\\
&= \left(\sum_{u\in V_1} d_{G_1}(u)\right)\left(\sum_{v\in V_2} d_{G_2}(v)\right) + 2n_1n_2(q_1+q_2) + (n_1n_2)^2\\
&= 4q_1q_2 + 2n_1n_2(q_1+q_2) + (n_1n_2)^2. \qquad (2.5)
\end{aligned}
$$

Adding (2.3), (2.4) and (2.5) we obtain formula (a). Formula (b) is a consequence of (a) together with Lemma 2.2. □

Example 2.1. The modified Schultz index of the complete split graph $CS_{q,p} = \overline{K}_p \nabla K_q$ can be computed using formula (a) of Theorem 2.1: $S^*(CS_{q,p}) = \frac{q}{2}((q-1)^3 + p^2(5q-1) + p(4q^2 - 8q + 2))$. In particular, $S^*(CS_{2,q}) = \frac{q}{2}(q^3 + 5q^2 + 7q - 1)$, and for a star with n vertices, $S_n = \overline{K}_{n-1}\nabla K_1$, $S^*(S_n) = 2n^2 - 5n + 3$.

2.2. **Cartesian product.** The cartesian product $G = G_1 \times G_2 = (V, E)$ of two disjoint graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ is the graph with vertex set $V = V_1 \times V_2$ where two vertices (u_1, u_2) and (v_1, v_2) are adjacent if they agree in one coordinate and are adjacent in the other, that is, if $u_1 = v_1$ and $u_2v_2 \in E_2$ or $u_1v_1 \in E_1$ and $u_2 = v_2$.

For $(u_1, u_2) \in V$ we have $d_G(u_1, u_2) = d_{G_1}(u_1) + d_{G_2}(u_2)$ and the distance between two vertices is $d_G((u_1, u_2), (v_1, v_2)) = d_{G_1}(u_1, v_1) + d_{G_2}(u_2, v_2)$.

Theorem 2.2. *The modified Schultz index of $G = G_1 \times G_2$ is given by*

$$S^*(G) = \sum_{\substack{i,j=1\\ i\neq j}}^{2} \Big(n_i^2 S^*(G_j) + 2q_i n_i S(G_j) + 4q_i^2 W(G_j) \Big).$$

Proof. Consider $A_1 = \{\{(u_1,u_2),(v_1,v_2)\} \subseteq V_1 \times V_2 : u_1 = v_1)\}$, $A_2 = \{\{(u_1,u_2),(v_1,v_2)\} \subseteq V_1 \times V_2 : u_2 = v_2)\}$ and $A_3 = \{\{(u_1,u_2),(v_1,v_2)\} \subseteq V_1 \times V_2 : u_1 \neq v_1, u_2 \neq v_2\}$. We have successively,

$$\begin{aligned} S^*_{A_1}(G) &= \sum_{w\in V_1} \sum_{\{u_2,v_2\}\subseteq V_2} \big(\left(d_{G_1}(w) + d_{G_2}(u_2)\right) \left(d_{G_1}(w) + d_{G_2}(v_2)\right) d_{G_2}(u_2,v_2) \big) \\ &= W(G_2) \sum_{w\in V_1} d_{G_1}(w)^2 + S(G_2) \sum_{w\in V_1} d_{G_1}(w) + \sum_{w\in V_1} S^*(G_2) \\ &= Z_1(G_1)\, W(G_2) + 2\, q_1 S(G_2) + n_1 S^*(G_2) \end{aligned}$$

and $S^*_{A_2}(G)$ is obtained in a similar way.

Using Lemma 2.1 we have

$$\begin{aligned} & S^*_{A_3}(G) = \\ & \sum_{\{x,y\}\in A_3} \left(d_{G_1}(u_1) + d_{G_2}(u_2)\right) \left(d_{G_1}(v_1) + d_{G_2}(v_2)\right) \left(d_{G_1}(u_1,v_1) + d_{G_2}(u_2,v_2)\right) \\ = & \sum_{\{x,y\}\in A_3} d_{G_1}(u_1)\, d_{G_1}(v_1)\, d_{G_1}(u_1,v_1) + \sum_{\{x,y\}\in A_3} d_{G_2}(u_2)\, d_{G_2}(v_2)\, d_{G_2}(u_2,v_2) \\ & + \sum_{\{x,y\}\in A_3} d_{G_2}(u_2) d_{G_2}(v_2)\, d_{G_1}(u_1,v_1) + \sum_{\{x,y\}\in A_3} d_{G_1}(u_1) d_{G_1}(v_1)\, d_{G_2}(u_2,v_2) \\ & + \sum_{\{x,y\}\in A_3} d_{G_1}(u_1)\, d_{G_2}(v_2)\, d_{G_1}(u_1,v_1) + \sum_{\{x,y\}\in A_3} d_{G_2}(u_2)\, d_{G_1}(v_1)\, d_{G_1}(u_1,v_1) \\ & + \sum_{\{x,y\}\in A_3} d_{G_1}(u_1)\, d_{G_2}(v_2)\, d_{G_2}(u_2,v_2) + \sum_{\{x,y\}\in A_3} d_{G_2}(u_2)\, d_{G_1}(v_1)\, d_{G_2}(u_2,v_2) \\ = & \; n_2\,(n_2-1)\, S^*(G_1) + n_1\,(n_1-1)\, S^*(G_2) + 2(2q_2^2 - \frac{1}{2} Z_1(G_2))W(G_1)) \\ & +2(2q_1^2 - \frac{1}{2} Z_1(G_1))W(G_2) + 2q_2(n_2-1)S(G_1) + 2q_1(n_1-1)S(G_2). \end{aligned}$$

As $\{A_1, A_2, A_3\}$ is a partition of the set of 2-sets of $V = V_1 \times V_2$, we obtain

$$\begin{aligned} S^*(G) &= S^*_{A_1}(G) + S^*_{A_2}(G) + S^*_{A_3}(G) \\ &= \sum_{\substack{i,j=1\\ i\neq j}}^{2} \Big(n_i^2 S^*(G_j) + 2q_i n_i S(G_j) + 4q_i^2 W(G_j) \Big). \end{aligned}$$

□

Example 2.2. The modified Schultz index of a 4-nanotube $P_n \times C_m$ (m even) is $S^*(P_n \times C_m) = \frac{m^3}{2}(1-2n)^2 + \frac{m^2}{3}(8n^3 - 12n^2 + 7n - 3)$; for the 4-nanotorus $C_k \times C_m$ (with k, m even), we have $S^*(C_k \times C_m) = 2k^2m^2(k+m)$ and for $P_n \times K_2$ (the ladder graph), $S^*(P_n \times K_2) = 6n^3 - 3n^2 - 2n$.

2.3. **Composition of graphs.** Let G_1 and G_2 be graphs with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2. The composition graph of G_1 and G_2, $G = G_1[G_2]$, is the graph with vertex set $V_1 \times V_2$ and (u_1, u_2) is adjacent to (v_1, v_2) whenever u_1 is adjacent to v_1 or $u_1 = v_1$ and u_2 is adjacent to v_2. For each $(u_1, u_2) \in V_1 \times V_2$, $d_G(u_1, u_2) = n_2 d_{G_1}(u_1) + d_{G_2}(u_2)$, and

$$d_G((u_1,u_2),(v_1,v_2)) = \begin{cases} 0 & \text{if } (u_1,u_2)=(v_1,v_2) \\ 1 & \text{if } u_1 = v_1 \text{ and } u_2v_2 \in E_2 \\ 2 & \text{if } u_1 = v_1 \text{ and } u_2v_2 \notin E_2 \\ d_{G_1}(u_1,v_1) & \text{if } u_1 \neq v_1 \end{cases}.$$

Theorem 2.3. *For $i = 1, 2$, let $G_i = (V_i, E_i)$ be a connected graph of order n_i and dimension q_i. Then the modified Schultz index of $G = G_1[G_2]$ is given by*

$$\begin{aligned} S^*(G) &= n_2^4 S^*(G_1) + 2n_2^2 q_2 S(G_1) + 4q_2^2 W(G_1) \\ &\quad + \left(n_2^3(n_2-1) - n_2^2 q_2\right) Z_1(G_1) - 2n_2 q_1 Z_1(G_2) \\ &\quad - n_1\left(Z_1(G_2) + Z_2(G_2)\right) + 8q_1q_2n_2(n_2-1) + 4n_1q_2^2. \end{aligned}$$

Proof. Let $A_1 = \{\{(u_1,u_2),(v_1,v_2)\} \subseteq V_1 \times V_2 \,:\, u_1 = v_1, u_2v_2 \in E_2\}$,
$A_2 = \{\{(u_1,u_2),(v_1,v_2)\} \subseteq V_1 \times V_2 \,:\, u_1 = v_1, u_2v_2 \notin E_2\}$,
$A_3 = \{\{(u_1,u_2),(v_1,v_2)\} \subseteq V_1 \times V_2 \,:\, u_1 \neq v_1, u_2 = v_2\}$ and
$A_4 = \{\{(u_1,u_2),(v_1,v_2)\} \subseteq V_1 \times V_2 \,:\, u_1 \neq v_1, u_2 \neq v_2\}$. Let $x = (w, u_2), y = (w, v_2) \in A_1$. Then

$$\begin{aligned} S^*_{A_1}(G) &= \sum_{\{x,y\}\in A_1} d_G(w,u_2)\, d_G(w,v_2)\, d_G((w,u_2),(w,v_2)) \\ &= \sum_{w\in V_1}\sum_{u_2v_2\in E_2} \big(d_{G_1}(w)n_2 + d_{G_2}(u_2)\big)\big(d_{G_1}(w)n_2 + d_{G_2}(v_2)\big) \\ &= n_2^2 \sum_{u_2v_2\in E_2}\sum_{w\in V_1} d^2_{G_1}(w) + n_2\sum_{w\in V_1} d_{G_1}(w) \sum_{u_2v_2\in E_2}\big(d_{G_2}(u_2) + d_{G_2}(v_2)\big) \\ &\quad + \sum_{w\in V_1}\sum_{u_2v_2\in E_2} d_{G_2}(u_2)d_{G_2}(v_2) \\ &= n_2^2 q_2 Z_1(G_1) + 2n_2q_1Z_1(G_2) + n_1Z_2(G_2). \end{aligned}$$

With $x = (w, u_2),\ y = (w, v_2) \in A_2$ and using Lemma 2.1 we have,

$$\begin{aligned} S^*_{A_2}(G) &= 2\sum_{w\in V_1}\sum_{u_2v_2\notin E_2} \big(d_{G_1}(w)n_2 + d_{G_2}(u_2)\big)\big(d_{G_1}(w)n_2 + d_{G_2}(v_2)\big) \\ &= 2n_2^2 \sum_{u_2v_2\notin E_2}\sum_{w\in V_1} d^2_{G_1}(w) + 2n_2\sum_{w\in V_1} d_{G_1}(w)\sum_{u_2v_2\notin E_2}\big(d_{G_2}(u_2) + d_{G_2}(v_2)\big) \\ &\quad + 2\sum_{w\in V_1}\sum_{u_2v_2\notin E_2} d_{G_2}(u_2)d_{G_2}(v_2) \\ &= 2n_2^2\left(\binom{n_2}{2} - q_2\right) Z_1(G_1) + 4n_2q_1\overline{Z}_1(G_2) + 2n_1\overline{Z}_2(G_2) \\ &= 2n_2^2\left(\binom{n_2}{2} - q_2\right) Z_1(G_1) + 4n_2q_1\big(2q_2(n_2-1) - Z_1(G_2)\big) \\ &\quad + 2n_1\big(2q_2^2 - \frac{1}{2}Z_1(G_2) - Z_2(G_2)\big) \end{aligned}$$

$$= 2\left(n_2^2\binom{n_2}{2} - n_2^2 q_2\right) Z_1(G_1) - 2(2q_1 n_2 + \frac{n_1}{2})Z_1(G_2)$$
$$-2n_1 Z_2(G_2) + 8q_1 q_2 n_2(n_2-1) + 4n_1 q_2^2.$$

With $x = (u_1, w)$, $y = (v_1, w) \in A_3$,

$$\begin{aligned}
S^*_{A_3}(G) &= n_2^2 \sum_{w\in V_2}\sum_{\{u_1,v_1\}\subseteq V_1} d_{G_1}(u_1)d_{G_1}(v_1)d_{G_1}(u_1,v_1) \\
&\quad + n_2 \sum_{w\in V_2} d_{G_2}(w) \sum_{\{u_1,v_1\}\subseteq V_1} \big((d_{G_1}(u_1)+d_{G_1}(v_1))\, d_{G_1}(u_1,v_1)\big) \\
&\quad + \sum_{w\in V_2} d_{G_2}(w)^2 \sum_{\{u_1,v_1\}\subseteq V_1} d_{G_1}(u_1,v_1) \\
&= n_2^3 S^*(G_1) + 2n_2 q_2 S(G_1) + Z_1(G_2)W(G_1).
\end{aligned}$$

For $x = (u_1, u_2)$, $y = (v_1, v_2) \in A_4$,

$$\begin{aligned}
S^*_{A_4}(G) &= \sum_{\{x,y\}\in A_4} (d_{G_1}(u_1)n_2 + d_{G_2}(u_2))(d_{G_1}(v_1)n_2 + d_{G_2}(v_2))d_{G_1}(u_1,v_1) \\
&= 2n_2^2 \sum_{\{u_2,v_2\}\subseteq V_2}\sum_{\{u_1,v_1\}\subseteq V_1} d_{G_1}(u_1)d_{G_1}(v_1)d_{G_1}(u_1,v_1) \\
&\quad + n_2 \sum_{u_2\in V_2}\sum_{v_2\in V_2\setminus\{u_2\}} d_{G_2}(u_2) \sum_{\{u_1,v_1\}\subseteq V_1} d_{G_1}(v_1)d_{G_1}(u_1,v_1) \\
&\quad + n_2 \sum_{v_2\in V_2}\sum_{u_2\in V_2\setminus\{v_2\}} d_{G_2}(v_2) \sum_{\{u_1,v_1\}\subseteq V_1} d_{G_1}(u_1)d_{G_1}(u_1,v_1) \\
&\quad + 2 \sum_{\{u_2,v_2\}\subseteq V_2} d_{G_2}(u_2)d_{G_2}(v_2) \sum_{\{u_1,v_1\}\subseteq V_1} d_{G_1}(u_1,v_1)
\end{aligned}$$

And by Lemma 2.1 we obtain

$$\begin{aligned}
S^*_{A_4}(G) &= 2n_2^2\binom{n_2}{2} S^*(G_1) + 2n_2(n_2-1)q_2 \sum_{\{u_1,v_1\}\subseteq V_1} (d_{G_1}(u_1)+d_{G_1}(v_1))\, d_{G_1}(u_1,v_1) \\
&\quad + 2\left(2q_2^2 - \frac{1}{2}Z_1(G_2)\right) W(G_1) \\
&= n_2^3\,(n_2-1)\, S^*(G_1) + 2n_2(n_2-1)q_2 S(G_1) + 4q_2^2 W(G_1) - Z_1(G_2)W(G_1).
\end{aligned}$$

Since $\{A_1, A_2, A_3, A_4\}$ is a partition of the set of 2-sets of $V = V_1 \times V_2$ then $S^*(G) = S^*_{A_1}(G) + S^*_{A_2}(G) + S^*_{A_3}(G) + S^*_{A_4}(G)$ and the result follows. □

Example 2.3. Composing paths and cycles with various small graphs one obtains classes of polymer-like graphs. For $G = P_n[K_p]$, we have $S^*(P_n[K_p]) = \frac{n^3p^2}{6}(1-3p)^2 + n^2p^3(1-3p) - p^2(6p^2 - 7p + 2) + \frac{np}{6}(42p^3 - 45p^2 + 20p - 3)$. In particular, for $P_n[K_2]$, the fence graph, $S^*(P_n[K_2]) = \frac{50}{3}n^3 - 40n^2 + \frac{193}{3}n - 48$.

2.4. **Subdivision of a graph.** The subdivision graph $G' = (V', E')$ of a graph G is the graph obtained from $G = (V, E)$ by inserting a new vertex of degree 2 in each edge of G. It follows immediately that $|V'| = |V| + |E|$ and $|E'| = 2|E|$. We define, for each $u \in V$, $D^*(u) = \sum_{e\in E} d^*_G(u, e)$ and $D^\diamond(G) = \sum_{u\in V} d_G(u)D^*(u)$.

Theorem 2.4. *Let $G = (V, E)$ be a connected graph of dimension q and $G' = (V', E')$ the subdivision graph of G. Then*

$$S^*(G') = 2S^*(G) + 8W(L(G)) + 4D^\diamond(G) + 4\,q^2.$$

Proof. For $u, v \in V'$,

$$d_{G'}(u,v) = \begin{cases} 2d_G(u,v), & \text{if } u,v \in V \\ 1 + 2d^*_G(u,e_v), & \text{if } u \in V, v \in V' \setminus V \\ 2 + 2D_G(e_u,e_v), & \text{if } u,v \in V' \setminus V \end{cases}$$

with $e_x \in E$ being the edge of G where a new vertex x is inserted.

In the following we use (1.1) to obtain

$$\begin{aligned} S^*(G') &= \sum_{\{u,v\}\subseteq V'} d_{G'}(u)d_{G'}(v)d_{G'}(u,v) \\ &= 2\sum_{\{u,v\}\subseteq V} d_G(u)d_G(v)d_G(u,v) + 2\sum_{u\in V}\sum_{v\in V'\setminus V} d_G(u)d_{G'}(u,v) \\ &\quad +4\sum_{\{u,v\}\subset V'\setminus V} d_{G'}(u,v) \\ &= 2S^*(G) + 2\sum_{u\in V}\sum_{e\in E} d_G(u)(1+2d^*_G(u,e)) + 4\sum_{\{e,f\}\subseteq E}(2+2D_G(e,f))) \\ &= 2S^*(G) + 4q^2 + 4D^\diamond(G) + 8\binom{q}{2} + 8W(L(G)) - 8\binom{q}{2} \\ &= 2S^*(G) + 8W(L(G)) + 4D^\diamond(G) + 4q^2. \end{aligned}$$

□

Example 2.4. Let G' be the subdivision graph of the complete graph K_n. From Theorem 2.4, it follows that $S^*(G') = 2S^*(K_n) + 8W(T_n) + 4D^\diamond(K_n) + 4\binom{n}{2}^2 = 2\binom{n}{2}\Big((n-1)^2 + 8\binom{n-1}{2} + 2\binom{n}{2}\Big) = 3n(n-1)^2(2n-3)$, with T_n being the line graph of K_n, that is, the triangular graph.

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