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SCHULTZ POLYNOMIALS OF COMPOSITE GRAPHS

Mehdi Eliasi, Bijan Taeri

For a connected graph G, the Schultz and modified Schultz polynomials, introduced by I. Gutman: *Some relations between distance-based polynomials of trees.* Bulletin, Classe des Sciences Mathématiques et Naturelles, Sciences mathématiques, Vol. CXXXI, **30** (2005) 1–7, are defined as $H_1(G,x) = \frac{1}{2}\sum\{(\delta_u+\delta_v)x^{d(u,v|G)} \mid u,v \in V(G), u \neq v\}$ and $H_2(G,x) = \frac{1}{2}\sum\{(\delta_u\delta_v)x^{d(u,v|G)} \mid u,v \in V(G), u \neq v\}$, respectively, where δ_u is the degree of vertex u, $d(u,v|G)$ is the distance between u and v and $V(G)$ is the vertex set of G. In this paper we find identities for the Schultz and modified Schultz polynomials of the sum, join and composition of graphs. As an application of our results we find the Schultz polynomial of C_4 nanotubes.

1. INTRODUCTION

Let G be a connected finite undirected graph without loops or multiple edges. Denote the vertex and edge sets of G by $V(G)$ and $E(G)$, respectively. The distance between two vertices u and v of G is denoted by $d(u,v|G)$ and it is defined as the number of edges in a shortest path connecting u and v. Distance is an important concept in graph theory and it has applications to computer science, chemistry, and a variety of other fields. The Wiener index of G is the sum of distances between all vertices of the graph G:

$$W(G) = \sum_{\{u,v\}\subset V(G)} d(u,v).$$

This index was introduced by the chemist Harold Wiener [**16**], about 60 years ago as a descriptor for explaining the boiling points of paraffins. A topological

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index is a real number related to a structural graph of a molecule. It does not depend on the labeling or pictorial representation of a graph. The WIENER index is one of the topological indices of a chemical compound that correlate with some of the physico-chemical properties of the compound (see for instance [**4**]). Also for a deeper discussion of the mathematical works we refer the reader to [**3**].

In [**8**] HARUO HOSOYA used polynomials to generate distance distributions for graphs. He introduced a distance-based polynomial and called it the WIENER polynomial.

$$H(G,x) = \frac{1}{2}\sum \{x^{d(u,v|G)} \mid u,v \in V(G), u \neq v\}.$$

The first derivative of $H(G,x)$ at $x = 1$ is equal to WIENER index of G.

The "molecular topological index" (SCHULTZ index) was introduced by HARRY SCHULTZ [**12**]. The SCHULTZ index is defined as

$$S(G) = \frac{1}{2}\sum \{(\delta_u + \delta_v)d(u,v|G) \mid u,v \in V(G), u \neq v\},$$

where δ_u is degree of vertex u. In addition to the chemical applications, the SCHULTZ index attracted some attention after it was discovered that in the case of trees it is closely related to the WIENER index [**11**]. In fact in [**11**] it is proved that if G is a tree on n vertices, then $S(G) = 4W(G) - n(n-1)$. KLAVZĂR and GUTMAN in [**10**] defined the modified SCHULTZ index as:

$$S^*(G) = \frac{1}{2}\sum \{\delta_u \delta_v d(u,v|G) \mid u,v \in V(G), u \neq v\}.$$

GUTMAN in [**5**] showed that if G is a tree on n vertices then $S^*(G) = 4W(G) - n(2n-1)$. GUTMAN [**6**] introduced new polynomials such that the their derivative at $x = 1$ are equal to the SCHULTZ and modified SCHULTZ index. He obtained some relationships between these polynomials and WIENER polynomial of trees. A similar work for hexagonal chains was done by SEN-PENG et. al. in [**14**].

Definition. *Let G be a connected graph. The Schultz polynomial of G is*:

$$H_1(G,x) = \frac{1}{2}\sum \{(\delta_u + \delta_v)x^{d(u,v|G)} \mid u,v \in V(G), u \neq v\}.$$

Also the modified Schultz polynomial of G is defined as:

$$H_2(G,x) = \frac{1}{2}\sum \{(\delta_u \delta_v)x^{d(u,v|G)} \mid u,v \in V(G), u \neq v\}.$$

In the original definition, the SCHULTZ (modified SCHULTZ) polynomial has the constant coefficient $|V(G)|$. In fact, one could include the case $u = v$ in the above definitions. Since the derivative of these polynomials are important, we may omit the constant terms.

STEVANOVIĆ [**13**] determined identities for the WIENER polynomial of the sum, join and composition of graphs and WEIGEN YAN et al. in [**15**] for some decorated graphs. In this paper, we find identities for the SCHULTZ (modified SCHULTZ) polynomial of sum, join and composition of graphs.

Throughout the paper we assume that $V_i = V(G_i)$, $n_i = |V_i|$ and $e_i = |E(G_i)|$, $i = 1, 2$. We use the very well known fact $\sum_{u\in V_i} \delta_u = 2e_i$ frequently. First we recall the definition of sum, join and composition of two graphs. Let G_1 and G_2 be two connected graphs.

I. The sum G_1+G_2 has the vertex set $V(G_1+G_2) = V_1\times V_2$ and two vertices (u_1, u_2) and (v_1, v_2) of $G_1 + G_2$ are adjacent if and only if $[u_1 = v_1$ and $(u_2, v_2) \in E(G_2)]$ or $[u_2 = v_2$ and $(u_1, v_1) \in E(G_1)]$.

II. The join $G_1\nabla G_2$ has the vertex set $V(G_1\nabla G_2) = V_1 \cup V_2$ and the edge set $E(G_1\nabla G_2) = E(G_1) \cup E(G_2) \cup \{(u_1, u_2) \mid u_1 \in V_1, u_2 \in V_2\}$.

III. The composition $G_1[G_2]$ has the vertex set $V(G_1[G_2]) = V_1 \times V_2$ and two vertices (u_1, u_2) and (v_1, v_2) of $G_1[G_2]$ are adjacent if and only if $[u_1 = v_1$ and $(u_2, v_2) \in E(G_2)]$ or $(u_1, v_1) \in E(G_1)$.

2. SCHULTZ AND MODIFIED SCHULTZ POLYNOMIALS OF COMPOSITE GRAPHS

We begin by obtaining a relation between the SCHULTZ polynomial of a sum of two graphs and their WIENER and SCHULTZ polynomials.

Theorem 1. *For two connected graphs G_1 and G_2 we have*

$$\begin{aligned}H_1(G_1 + G_2, x) = {} & 2H_1(G_1, x)H(G_2, x) + 2H(G_1, x)H_1(G_2, x)\\ & +n_2H_1(G_1, x) + 4e_2H(G_1, x) + n_1H_1(G_2, x) + 4e_1H(G_2, x).\end{aligned}$$

Proof. Suppose that $u = (u_1, u_2)$ and $v = (v_1, v_2)$. It is easy to see that $\delta_u = \delta_{u_1} + \delta_{u_2}$ and according to the proof of Theorem 1 in [**13**] we have $d(u, v|G_1+G_2) = d(u_1, v_1|G_1) + d(u_2, v_2|G_2)$. Hence

$$\begin{aligned}H_1(G_1 + G_2, x) &= \frac{1}{2}\sum \{(\delta_u + \delta_v)x^{d(u,v|G_1+G_2)} \mid u, v \in V(G_1 + G_2), u \neq v\}\\
&= \frac{1}{2}\sum \{(\delta_{u_1} + \delta_{u_2} + \delta_{v_1} + \delta_{v_2})x^{d(u_1,v_1|G_1)+d(u_2,v_2|G_2)} \mid\\
&\qquad\qquad u_1, v_1 \in V_1, u_2, v_2 \in V_2, u_1 \neq v_1 \text{ or } u_2 \neq v_2\}\\
&= \frac{1}{2}\sum_{u_1\neq v_1}\sum_{u_2\neq v_2}(\delta_{u_1} + \delta_{v_1} + \delta_{u_2} + \delta_{v_2})x^{d(u_1,v_1|G_1)}x^{d(u_2,v_2|G_2)}\\
&\quad + \frac{1}{2}\sum_{u_1\neq v_1}\sum_{u_2=v_2}(\delta_{u_1} + \delta_{v_1} + \delta_{u_2} + \delta_{v_2})x^{d(u_1,v_1|G_1)}x^{d(u_2,v_2|G_2)}\\
&\quad + \frac{1}{2}\sum_{u_1=v_1}\sum_{u_2\neq v_2}(\delta_{u_1} + \delta_{v_1} + \delta_{u_2} + \delta_{v_2})x^{d(u_1,v_1|G_1)}x^{d(u_2,v_2|G_2)}\end{aligned}$$

$$= \Big(\frac{1}{2}\sum_{u_1\neq v_1}\sum_{u_2\neq v_2}(\delta_{u_1}+\delta_{v_1})x^{d(u_1,v_1|G_1)}x^{d(u_2,v_2|G_2)}$$
$$+\frac{1}{2}\sum_{u_1\neq v_1}\sum_{u_2\neq v_2}(\delta_{u_2}+\delta_{v_2})x^{d(u_1,v_1|G_1)}x^{d(u_2,v_2|G_2)}\Big)$$
$$+\frac{1}{2}\sum_{u_1\neq v_1}\sum_{u_2\in V_2}(\delta_{u_1}+\delta_{v_1}+2\delta_{u_2})x^{d(u_1,v_1|G_1)}$$
$$+\frac{1}{2}\sum_{u_1\in V_1}\sum_{u_2\neq v_2}(2\delta_{u_1}+\delta_{u_2}+\delta_{v_2})x^{d(u_2,v_2|G_2)}$$
$$= \Big(2H_1(G_1,x)H(G_2,x)+2H(G_1,x)H_1(G_2,x)\Big)$$
$$+n_2H_1(G_1,x)+4e_2H(G_1,x)+n_1H_1(G_2,x)+4e_1H(G_2,x),$$

which completes the proof. □

The next theorem is analogous to Theorem 1 and expresses the relation between the modified Schultz polynomial of a sum of two graphs and their Wiener, Schultz and modified Schultz polynomials.

Theorem 2. *For each two connected graphs G_1 and G_2 we have*

$$H_2(G_1+G_2,x)=2H_2(G_1,x)H(G_2,x)+H_1(G_1,x)H_1(G_2,x)+2H(G_1,x)H_2(G_2,x)$$
$$+n_2H_2(G_1,x)+2e_2H_1(G_1,x)+D_2H(G_1,x)$$
$$+n_1H_2(G_2,x)+2e_1H_1(G_2,x)+D_1H(G_2,x),$$

where $D_1=\sum_{u_1\in V_1}\delta_{u_1}^2$ and $D_2=\sum_{u_2\in V_2}\delta_{u_2}^2$.

Proof. As in the proof of Theorem 1 we have

$$H_2(G_1+G_2,x)=\frac{1}{2}\sum\{\delta_u\delta_v x^{d(u,v|G_1+G_2)}\mid u,v\in V(G_1+G_2),u\neq v\}$$
$$=\frac{1}{2}\sum\{(\delta_{u_1}+\delta_{u_2})(\delta_{v_1}+\delta_{v_2})x^{d(u_1,v_1|G_1)+d(u_2,v_2|G_2)}\mid$$
$$u_1,v_1\in V_1,u_2,v_2\in V_2,u_1\neq v_1 \text{ or } u_2\neq v_2\}$$
$$=\frac{1}{2}\sum_{u_1\neq v_1}\sum_{u_2\neq v_2}(\delta_{u_1}+\delta_{u_2})(\delta_{v_1}+\delta_{v_2})x^{d(u_1,v_1|G_1)}x^{d(u_2,v_2|G_2)}$$
$$+\frac{1}{2}\sum_{u_1\neq v_1}\sum_{u_2=v_2}(\delta_{u_1}+\delta_{u_2})(\delta_{v_1}+\delta_{v_2})x^{d(u_1,v_1|G_1)}x^{d(u_2,v_2|G_2)}$$
$$+\frac{1}{2}\sum_{u_1=v_1}\sum_{u_2\neq v_2}(\delta_{u_1}+\delta_{u_2})(\delta_{v_1}+\delta_{v_2})x^{d(u_1,v_1|G_1)}x^{d(u_2,v_2|G_2)}.$$

Expanding the three last sums we have

$$\begin{aligned}
H_2(G_1+G_2,x) &= \Big(\frac{1}{2}\sum_{u_1\neq v_1}\sum_{u_2\neq v_2}\delta_{u_1}\delta_{v_1}x^{d(u_1,v_1|G_1)}x^{d(u_2,v_2|G_2)}\\
&+\frac{1}{2}\sum_{u_1\neq v_1}\sum_{u_2\neq v_2}\delta_{u_1}\delta_{v_2}x^{d(u_1,v_1|G_1)}x^{d(u_2,v_2|G_2)}\\
&+\frac{1}{2}\sum_{u_1\neq v_1}\sum_{u_2\neq v_2}\delta_{u_2}\delta_{v_1}x^{d(u_1,v_1|G_1)}x^{d(u_2,v_2|G_2)}\\
&+\frac{1}{2}\sum_{u_1\neq v_1}\sum_{u_2\neq v_2}\delta_{u_2}\delta_{v_2}x^{d(u_1,v_1|G_1)}x^{d(u_2,v_2|G_2)}\Big)\\
&+\Big(\frac{1}{2}\sum_{u_1\neq v_1}\sum_{u_2\in V_2}\delta_{u_1}\delta_{v_1}x^{d(u_1,v_1|G_1)}+\frac{1}{2}\sum_{u_1\neq v_1}\sum_{u_2\in V_2}\delta_{u_1}\delta_{u_2}x^{d(u_1,v_1|G_1)}\\
&+\frac{1}{2}\sum_{u_1\neq v_1}\sum_{u_2\in V_2}\delta_{u_2}\delta_{v_1}x^{d(u_1,v_1|G_1)}+\frac{1}{2}\sum_{u_1\neq v_1}\sum_{u_2\in V_2}\delta_{u_2}^2x^{d(u_1,v_1|G_1)}\Big)\\
&+\Big(\frac{1}{2}\sum_{u_1\in V_1}\sum_{u_2\neq v_2}\delta_{u_1}^2x^{d(u_2,v_2|G_2)}+\frac{1}{2}\sum_{u_1\in V_1}\sum_{u_2\neq v_2}\delta_{u_1}\delta_{v_2}x^{d(u_2,v_2|G_2)}\\
&+\frac{1}{2}\sum_{u_1\in V_1}\sum_{u_2\neq v_2}\delta_{u_2}\delta_{u_1}x^{d(u_2,v_2|G_2)}+\frac{1}{2}\sum_{u_1\in V_1}\sum_{u_2\neq v_2}\delta_{u_2}\delta_{v_2}x^{d(u_2,v_2|G_2)}\Big).
\end{aligned}$$

But $\sum_{u_1\neq v_1}\delta_{u_1}x^{d(u_1,v_1|G_1)}=H_1(G_1,x)$ and similarly $\sum_{u_2\neq v_2}\delta_{u_2}x^{d(u_2,v_2|G_2)}=H_1(G_2,x)$. Using these facts we obtain that

$$\begin{aligned}
H_2(G_1+G_2,x) &= \Big(2H_2(G_1,x)H(G_2,x)+\frac{1}{2}H_1(G_1,x)H_1(G_2,x)\\
&\quad+\frac{1}{2}H_1(G_2,x)H_1(G_1,x)+2H(G_1,x)H_2(G_2,x)\Big)\\
&\quad+\Big(n_2H_2(G_1,x)+e_2H_1(G_1,x)+e_2H_1(G_1,x)+D_2H(G_1,x)\Big)\\
&\quad+\Big(D_1H(G_2,x)+e_1H_1(G_2,x)+e_1H_1(G_2,x)+n_1H_2(G_2,x)\Big)\\
&= 2H_2(G_1,x)H(G_2,x)+H_1(G_1,x)H_1(G_2,x)\\
&\quad+2H(G_1,x)H_2(G_2,x)+n_2H_2(G_1,x)+2e_2H_1(G_1,x)\\
&\quad+D_2H(G_1,x)+n_1H_2(G_2,x)+2e_1H_1(G_2,x)+D_1H(G_2,x).
\end{aligned}$$

This completes the proof. □

From now on for connected graphs G_1 and G_2, we consider the sets A_1, A_2, B_1 and B_2 as follows:

$$\begin{aligned}
A_1 &:= \{\{u,v\}\subseteq V_1 \mid u\neq v,\ uv\notin E(G_1)\},\ A_2:=\{\{z,t\}\subseteq V_2\mid z\neq t, zt\notin E(G_2)\}\\
B_1 &:= \{\{u,v\}\subseteq V_1 \mid u\neq v,\ uv\in E(G_1)\},\ B_2:=\{\{z,t\}\subseteq V_2\mid z\neq t, zt\in E(G_2)\}.
\end{aligned}$$

Now we prove two theorems that characterize the SCHULTZ and modified SCHULTZ polynomials of the join $G_1 \nabla G_2$. Since two vertices of $G_1 \nabla G_2$ are either adjacent or at distance two, the SCHULTZ and modified SCHULTZ polynomials of $G_1 \nabla G_2$ are polynomials of degree 2. So it remains to compute the coefficients of x and x^2. From now on we put $\overline{e_i} = \binom{n_i}{2} - e_i$, $i = 1, 2$.

Theorem 3. *Let G_1 and G_2 be connected graphs. Then*

$$\begin{aligned} H_1(G_1 \nabla G_2, x) = \Big[& \sum_{\{u,v\} \in A_1} (\delta_u + \delta_v) + 2n_2 \overline{e_1} + \sum_{\{z,t\} \in A_2} (\delta_u + \delta_v) + 2n_1 \overline{e_2} \Big] x^2 \\ + \Big[& \sum_{\{u,v\} \in B_1} (\delta_u + \delta_v) + \sum_{\{z,t\} \in B_2} (\delta_z + \delta_t) \\ & + 2n_1 e_2 + 42 n_2 e_1 + 2n_1 3_2 + (n_1 + n_2) n_1 n_2 \Big] x. \end{aligned}$$

Proof. Two vertices of $G_1 \nabla G_2$ are either adjacent or have distance two. The pairs of vertices having distance two are in $A_1 \cup A_2$. Also if δ_u is the degree of u in G_1 then the degree of u in $G_1 \nabla G_2$ is $\delta_u + n_2$. Similarly each $z \in V_2$ has degree $\delta_z + n_1$ in $G_1 \nabla G_2$. Hence the coefficient of x^2 in $H_1(G_1 \nabla G_2, x)$ is

$$\begin{aligned} & \sum_{\{u,v\} \in A_1} (\delta_u + n_2 + \delta_v + n_2) + \sum_{\{z,t\} \in A_2} (\delta_z + n_1 + \delta_t + n_1) \\ & = \sum_{\{u,v\} \in A_1} (\delta_u + \delta_v) + \sum_{\{u,v\} \in A_1} 2n_2 + \sum_{\{z,t\} \in A_2} (\delta_z + \delta_t) + \sum_{\{z,t\} \in A_2} 2n_1 \\ & = \sum_{\{u,v\} \in A_1} (\delta_u + \delta_v) + 2n_2 \overline{e_1} + \sum_{\{z,t\} \in A_2} (\delta_u + \delta_v) + 2n_1 \overline{e_2}. \end{aligned}$$

Similarly the coefficient of x in $H_1(G_1 \nabla G_2, x)$ is

$$\begin{aligned} & \sum_{\{u,v\} \in B_1} (\delta_u + n_2 + \delta_v + n_2) + \sum_{\{z,t\} \in B_2} (\delta_z + n_1 + \delta_t + n_1) + \sum_{u \in V_1, z \in V_2} (\delta_u + n_2 + \delta_z + n_1) \\ & = \sum_{\{u,v\} \in B_1} (\delta_u + \delta_v) + \sum_{\{u,v\} \in B_1} 2n_2 + \sum_{\{z,t\} \in B_2} (\delta_z + \delta_t) \\ & \quad + \sum_{u \in V_1, t \in V_2} (\delta_u + \delta_t) + \sum_{\{z,t\} \in B_2} 2n_1 + \sum_{u \in V_1, t \in V_2} (n_1 + n_2) \\ & = \sum_{\{u,v\} \in B_1} (\delta_u + \delta_v) + \sum_{\{z,t\} \in B_2} (\delta_z + \delta_t) + 2n_1 e_2 + 4n_2 e_1 + 2n_1 e_2 + (n_1 + n_2) n_1 n_2. \end{aligned}$$

This completes the proof. □

In the same way we can find an identity for the modified SCHULTZ polynomial of $G_1 \nabla G_2$.

Theorem 4. *Let G_1 and G_2 be connected graphs. Then*

$$H_2(G_1\nabla G_2,x)=\Bigg[\sum_{\{u,v\}\in A_1}\delta_u\delta_v+n_2\sum_{\{u,v\}\in A_1}(\delta_u+\delta_v)+n_2^2\,\overline{e_1}+\sum_{\{z,t\}\in A_2}\delta_z\delta_t$$
$$+n_1\sum_{\{z,t\}\in A_2}(\delta_z+\delta_t)+n_1^2\,\overline{e_2}\Bigg]x^2$$
$$+\Bigg[\sum_{\{u,v\}\in B_1}\delta_u\delta_v+n_2\sum_{\{u,v\}\in B_1}(\delta_u+\delta_v)+n_2^2e_1+\sum_{\{z,t\}\in B_2}\delta_z\delta_t$$
$$+n_1\sum_{\{z,t\}\in B_2}(\delta_z+\delta_t)+n_1^2e_2+4e_1e_2+2e_1n_1n_2+2e_2n_1n_2+n_1^2n_2^2\Bigg]x.$$

Proof. We follow the proof of Theorem 3. The coefficient of x^2 in $H_2(G_1\nabla G_2,x)$ is equal to

$$\sum_{\{u,v\}\in A_1}(\delta_u+n_2)(\delta_v+n_2)+\sum_{\{z,t\}\in A_2}(\delta_z+n_1)(\delta_t+n_1)$$
$$=\sum_{\{u,v\}\in A_1}\delta_u\delta_v+\sum_{\{u,v\}\in A_1}(\delta_u+\delta_v)n_2+\sum_{\{u,v\}\in A_1}n_2^2+\sum_{\{z,t\}\in A_2}\delta_z\delta_t$$
$$+\sum_{\{z,t\}\in A_2}(\delta_z+\delta_t)n_1+\sum_{\{z,t\}\in A_2}n_1^2$$
$$=\sum_{\{u,v\}\in A_1}\delta_u\delta_v+n_2\sum_{\{u,v\}\in A_1}(\delta_u+\delta_v)+n_2^2\,\overline{e_1})+\sum_{\{z,t\}\in A_2}\delta_z\delta_t$$
$$+n_1\sum_{\{z,t\}\in A_2}(\delta_z+\delta_t)+n_1^2\,\overline{e_2}.$$

Similarly the coefficient of x in $H_1(G_1\nabla G_2,x)$ is

$$\sum_{\{u,v\}\in B_1}(\delta_u+n_2)(\delta_v+n_2)+\sum_{\{z,t\}\in B_2}(\delta_z+n_1)(\delta_t+n_1)+\sum_{u\in V_1,z\in V_2}(\delta_u+n_2)(\delta_z+n_1)$$
$$=\sum_{\{u,v\}\in B_1}\delta_u\delta_v+\sum_{\{u,v\}\in B_1}(\delta_u+\delta_v)n_2+\sum_{\{u,v\}\in B_1}n_2^2+\sum_{\{z,t\}\in B_2}\delta_z\delta_t$$
$$+\sum_{\{z,t\}\in B_2}(\delta_z+\delta_t)n_1+\sum_{\{z,t\}\in B_2}n_1^2+\sum_{u\in V_1,z\in V_2}\delta_u\delta_z$$
$$+\sum_{u\in V_1,z\in V_2}\delta_un_1+\sum_{u\in V_1,z\in V_2}\delta_zn_2+\sum_{u\in V_1),z\in V_2}n_1n_2$$
$$=\sum_{\{u,v\}\in B_1}\delta_u\delta_v+n_2\sum_{\{u,v\}\in B_1}(\delta_u+\delta_v)+n_2^2e_1+\sum_{\{z,t\}\in B_2}\delta_z\delta_t$$
$$+n_1\sum_{\{z,t\}\in B_2}(\delta_z+\delta_t)+n_1^2e_2+4e_1e_2+2e_1n_1n_2+2e_2n_1n_2+n_1^2n_2^2.$$

This completes the proof. □

In the next theorem we find an identity for the SCHULTZ and modified SCHULTZ polynomials of the composition $G_1[G_2]$.

Theorem 5. *Let G_1 and G_2 be connected graphs. Then*

$$H_1(G_1[G_2],x) = n_2 3H_1(G_1,x) + 4n_2e_2H(G_1,x) + \left[4n_2e_1\overline{e_2} + n_1 \sum_{\{u_2,v_2\}\in A_2} (\delta_{u_2} + \delta_{v_2})\right]x^2 + \left[4n_2e_1e_2 + n_1 \sum_{\{u_2,v_2\}\in B_2} (\delta_{u_2} + \delta_{v_2})\right]x.$$

Proof. Suppose that $u = (u_1, u_2)$ and $v = (v_1, v_2)$ be vertices of $G_1[G_2]$. Then

$$d(u,v|G_1[G_2]) = \begin{cases} d(u_1,v_1|G_1) & \text{if} \quad u_1 \neq v_1 \\ 1 & \text{if} \quad u_1 = v_1 \quad \text{and} \quad (u_2,v_2) \in E(G_2) \\ 2 & \text{if} \quad u_1 = v_1 \quad \text{and} \quad (u_2,v_2) \notin E(G_2). \end{cases}$$

Also $\delta_{(u_1,u_2)} = n_2\delta_{u_1} + \delta_{u_2}$ and $\delta_{(v_1,v_2)} = n_2\delta_{v_1} + \delta_{v_2}$. So

$$\begin{aligned}
H_1(G_1[G_2],x) &= \frac{1}{2}\sum\{(\delta_u + \delta_v)x^{d(u,v|G_1[G_2])} \mid u,v \in V(G_1[G_2]), u \neq v\} \\
&= \frac{1}{2}\sum\{(n_2\delta_{u_1} + \delta_{u_2} + n_2\delta_{v_1} + \delta_{v_2})x^{d(u_1,v_1|G_1)} \mid u_1,v_1 \in V_1, u_2,v_2 \in V_1, u_1 \neq v_1\} \\
&\quad + \frac{1}{2}\sum\{(n_2\delta_{u_1} + \delta_{u_2} + n_2\delta_{v_1} + \delta_{v_2})x^2 \mid u_1 = v_1, (u_2,v_2) \notin E(G_2)\} \\
&\quad + \frac{1}{2}\sum\{(n_2\delta_{u_1} + \delta_{u_2} + n_2\delta_{v_1} + \delta_{v_2})x \mid u_1 = v_1, (u_2,v_2) \in E(G_2)\} \\
&= \frac{1}{2}\sum_{u_2\in V_2}\sum_{v_2\in V_2}\sum_{u_1\neq v_1}(n_2\delta_{u_1} + \delta_{u_2} + n_2\delta_{v_1} + \delta_{v_2})x^{d(u_1,v_1|G_1)} \\
&\quad + \frac{1}{2}\sum_{u_1\in V_1}\sum_{\{u_2,v_2\}\in A_2}(2\delta_{u_1}n_2 + \delta_{u_2} + \delta_{v_2})x^2 \\
&\quad + \frac{1}{2}\sum_{u_1\in V_1}\sum_{\{u_2,v_2\}\in B_2}(2\delta_{u_1}n_2 + \delta_{u_2} + \delta_{v_2})x \\
&= \left[\frac{1}{2}\sum_{u_2\in V_2}\sum_{v_2\in V_2}\sum_{u_1\neq v_1}n_2(\delta_{u_1} + \delta_{v_1})x^{d(u_1,v_1|G_1)} \right.\\
&\quad \left. + \frac{1}{2}\sum_{u_2\in V_2}\sum_{v_2\in V_2}\sum_{u_1\neq v_1}(\delta_{u_2} + \delta_{v_2})x^{d(u_1,v_1|G_1)}\right] \\
&\quad + \left[\frac{1}{2}\sum_{u_1\in V_1}\sum_{\{u_2,v_2\}\in A_2}2n_2\delta_{u_1} + \frac{1}{2}\sum_{u_1\in V_1}\sum_{\{u_2,v_2\}\in A_2}(\delta_{u_2} + \delta_{v_2})\right]x^2 \\
&\quad + \frac{1}{2}\sum_{u_1\in V_1}\sum_{\{u_2,v_2\}\in B_2}2n_2\delta_{u_1} + \frac{1}{2}\sum_{u_1\in V_1}\sum_{\{u_2,v_2\}\in B_2}(\delta_{u_2} + \delta_{v_2})\Big]x \\
&= \left[n_2^3H_1(G_1,x) + 4n_2e_2H(G_1,x)\right] + \left[4n_2e_1\overline{e_2} + n_1\sum_{\{u_2,v_2\}\in A_2}(\delta_{u_1} + \delta_{u_2})\right]x^2 \\
&\quad + \left[4n_2e_1e_2 + n_1\sum_{\{u_2,v_2\}\in B_2}(\delta_{u_1} + \delta_{u_2})\right]x.
\end{aligned}$$

So the theorem is proved. □

Now we prove the final theorem of this section that expresses the modified SCHULTZ polynomial of the composition graph $G_1[G_2]$.

Theorem 6. *For each two connected graphs G_1 and G_2 we have*

$$\begin{aligned}H_2(G_1[G_2],x) = &\Big[n_2^2 H_2(G_1,x) + n_2^3 H_1(G_1,x) + 4e_2^2 H(G_1,x)\Big]\\ &+\Big[n_2^2 D_1\overline{e_2} + 2n_2e_1 \sum_{\{u_2,v_2\}\in A_2} (\delta_{u_2}+\delta_{v_2}) + n_1 \sum_{\{u_2,v_2\}\in A_2} \delta_{u_2}\delta_{v_2}\Big]x^2\\ &+\Big[n_2^2 e_2 D_1 + 2n_2e_1 \sum_{\{u_2,v_2\}\in B_2} (\delta_{u_2}+\delta_{v_2}) + n_1 \sum_{\{u_2,v_2\}\in B_2} \delta_{u_2}\delta_{v_2}\Big]x,\end{aligned}$$

where $D_1 = \sum_{u_1\in V_1} \delta_{u_1}^2$.

Proof. We follow the proof of Theorem 5. We have

$$\begin{aligned}H_2(G_1[G_2],x) &= \frac{1}{2}\sum\{\delta_u\delta_v x^{d(u,v|G_1[G_2])} \mid u,v\in V(G_1[G_2]),\ u\neq v\}\\ &= \frac{1}{2}\sum\{(n_2\delta_{u_1}+\delta_{u_2})(n_2\delta_{v_1}+\delta_{v_2})x^{d(u_1,v_1|G_1)} \mid u_1,v_1\in V_1, u_2,v_2\in V_1, u_1\neq v_1\}\\ &\quad+\frac{1}{2}\sum\{(n_2\delta_{u_1}+\delta_{u_2})(n_2\delta_{v_1}+\delta_{v_2})x^2 \mid u_1=v_1,\ (u_2,v_2)\notin E(G_2)\}\\ &\quad+\frac{1}{2}\sum\{(n_2\delta_{u_1}+\delta_{u_2})(n_2\delta_{v_1}+\delta_{v_2})x \mid u_1=v_1,\ (u_2,v_2)t\in E(G_2)\}\\ &= \frac{1}{2}\sum_{u_2\in V_2}\sum_{v_2\in V_2}\sum_{u_1\neq v_1}(n_2\delta_{u_1}+\delta_{u_2})(n_2\delta_{v_1}+\delta_{v_2})x^{d(u_1,v_1|G_1)}\\ &\quad+\frac{1}{2}\sum_{u_1\in V_1}\sum_{\{u_2,v_2\}\in A_2}(n_2\delta_{u_1}+\delta_{u_2})(n_2\delta_{u_1}+\delta_{v_2})x^2\\ &\quad+\frac{1}{2}\sum_{u_1\in V_1}\sum_{\{u_2,v_2\}\in B_2}(n_2\delta_{u_1}+\delta_{u_2})(n_2\delta_{u_1}+\delta_{v_2})x\\ &= \frac{1}{2}\Big[\sum_{u_2\in V_2}\sum_{v_2\in V_2}\sum_{u_1\neq v_1} n_2^2\delta_{u_1}\delta_{v_1}x^{d(u_1,v_1|G_1)} + \sum_{u_2\in V_2}\sum_{v_2\in V_2}\sum_{u_1\neq v_1} n_2\delta_{u_1}\delta_{v_2}x^{d(u_1,v_1|G_1)}\\ &\quad+\sum_{u_2\in V_2}\sum_{v_2\in V_2}\sum_{u_1\neq v_1} n_2\delta_{u_2}\delta_{v_1}x^{d(u_1,v_1|G_1)} + \sum_{u_2\in V_2}\sum_{v_2\in V_2}\sum_{u_1\neq v_1} \delta_{u_2}\delta_{v_2}x^{d(u_1,v_1|G_1)}\Big]\\ &\quad+\frac{1}{2}\Big[\sum_{u_1\in V_1}\sum_{\{u_2,v_2\}\in A_2} n_2^2\delta_{u_1}^2 + \sum_{u_1}\sum_{\{u_2,v_2\}\in A_2} n_2\delta_{u_1}(\delta_{u_2}+\delta_{v_2})\\ &\qquad\qquad+\sum_{u_1\in V_1}\sum_{\{u_2,v_2\}\in A_2}\delta_{u_2}\delta_{v_2}\Big]x^2\end{aligned}$$

$$+\frac{1}{2}\Bigg[\sum_{u_1\in V_1}\sum_{\{u_2,v_2\}\in B_2} n_2^2\delta_{u_1}^2+\sum_{u_1\in V_1}\sum_{\{u_2,v_2\}\in B_2} n_2\delta_{u_1}(\delta_{u_2}+\delta_{v_2})$$

$$+\sum_{u_1\in V_1}\sum_{\{u_2,v_2\}\in B_2}\delta_{u_2}\delta_{v_2}\Bigg]x$$

$$=\Big[n_2^2H_2(G_1,x)+\frac{1}{2}n_2^3H_1(G_1,x)+\frac{1}{2}n_2^3H_1(G_1,x)+2e_2^2H(G_1,x)\Big]$$

$$+\Big[n_2^2D_1\overline{e_2}+2n_2e_1\sum_{\{u_2,v_2\}\in A_2}(\delta_{u_2}+\delta_{v_2})+n_1\sum_{\{u_2,v_2\}\in A_2}\delta_{u_2}\delta_{v_2}\Big]x^2$$

$$+\Big[n_2^2D_1e_2+2n_2e_1\sum_{\{u_2,v_2\}\in B_2}(\delta_{u_2}+\delta_{v_2})+n_1\sum_{\{u_2,v_2\}\in B_2}\delta_{u_2}\delta_{v_2}\Big]x,$$

which proves the desired statement. □

At the end we present some applications of the results obtained in the paper.

EXAMPLE 1. Let $G=P_n$ be the path with n vertices. Then it is easy to see that

$$H(G,x)=x^{n-1}+2x^{n-2}+\cdots+(n-1)x$$

$$H_1(G,x)=2x^{n-1}+\sum_{k=1}^{n-2}[6+4(n-k-2)]x^k$$

$$H_2(G,x)=x^{n-1}+\sum_{k=1}^{n-2}[4+4(n-k-2)]x^k.$$

By Theorem 1 we can see that

$$H_1(P_n+P_m,x)=\frac{2}{(x-1)^4}\Big(4x^{m+n+2}+4x^{m+n+1}-3nx^{m+3}-3mx^{n+3}$$
$$-(n+4)x^{m+2}-(m+4)x^{n+2}+(3n-4)x^{m+1}+(3m-4)x^{n+1}+nx^m$$
$$+mx^n+(m+n)x^4-(n+m-8mn)x^3+(4+7n+7m-16mn)x^2$$
$$-(7n+7m-4-8mn)x\Big).$$

Also the SCHULTZ index of P_n+P_m is

$$S(P_n+P_m)=\frac{1}{3}mn(-2n^2-2m^2-6mn-m-n+4+4m^2n+4mn^2).$$

EXAMPLE 2. Let $G=P_n+C_m$, where C_m is the cycle with m vertices. Then $G=TUC_4[m,n]$ is a C_4-nanotube (see [**9**]). It is easy to see that

$$H(C_n,x)=\begin{cases}(nx^{[\frac{n}{2}]}+nx^{[\frac{n}{2}]-1}+\cdots+nx) & \text{if } n \text{ is odd}\\ \Big(\frac{n}{2}x^{[\frac{n}{2}]}+nx^{[\frac{n}{2}]-1}+\cdots+nx\Big) & \text{if } n \text{ is even}\end{cases}$$

$$=\begin{cases}(x^{[\frac{n}{2}]}t-t) & \text{if } n \text{ is odd}\\ n\Big(x^{[\frac{n}{2}]}\Big(t-\frac{1}{2}\Big)-t\Big) & \text{if } n \text{ is even}\end{cases}$$

where $t = \dfrac{x}{x-1}$, and $H_1(C_n, x) = 4H(C_n, x)$. Therefore by Theorem 1, if m is odd, we have

$$\begin{aligned}H_1(G,x) &= 2\Big(2x^{n-1} + \sum_{k=1}^{n-2}[6+4(n-k-2)]x^k\Big)\Big(m(x^{\left[\frac{m}{2}\right]}t - t)\Big)\\ &+2\Big(x^{n-1} + 2x^{n-2} + \cdots + (n-1)x\Big)\Big(4m(x^{\left[\frac{m}{2}\right]}t - t)\Big)\\ &+m\Big(2x^{n-1} + \sum_{k=1}^{n-2}[6+4(n-k-2)]x^k\Big)\\ &+4(m-1)\Big(x^{n-1} + 2x^{n-2} + \cdots + (n-1)x\Big)\\ &+4n\Big(m(x^{\left[\frac{m}{2}\right]}t - t)\Big) + 4(n-1)\Big(m(x^{\left[\frac{m}{2}\right]}t - t)\Big)\end{aligned}$$

and if m is even

$$\begin{aligned}H_1(G,x) &= 2\Big(2x^{n-1} + \sum_{k=1}^{n-2}[6+4(n-k-2)]x^k\Big)\Big(m\Big(x^{\left[\frac{m}{2}\right]}\Big(t-\frac{1}{2}\Big) - t\Big)\Big)\\ &+2\Big(x^{n-1} + 2x^{n-2} + \cdots + (n-1)x\Big)\Big(4m\Big(x^{\left[\frac{m}{2}\right]}\Big(t-\frac{1}{2}\Big) - t\Big)\Big)\\ &+m\Big(2x^{n-1} + \sum_{k=1}^{n-2}[6+4(n-k-2)]x^k\Big)\\ &+4(m-1)\Big(x^{n-1} + 2x^{n-2} + \cdots + (n-1)x\Big)\\ &+4n\Big(m\Big(x^{\left[\frac{m}{2}\right]}\Big(t-\frac{1}{2}\Big) - t\Big)\Big) + 4(n-1)\Big(m\Big(x^{\left[\frac{m}{2}\right]}\Big(t-\frac{1}{2}\Big) - t\Big)\Big).\end{aligned}$$

Now let $G = C_k + C_m$. Then $G = T_{k,m,C_4}$ is a C_4-nanotori, when m and k are odd, (see [**2**]). By Theorem 1 we obtain that

$$\begin{aligned}H_1(T_{k,m,C_4},x) &= 2\Big(4k\Big(x^{\left[\frac{k}{2}\right]}\Big(t-\frac{1}{2}\Big) - t\Big)\Big)\Big(m\Big(x^{\left[\frac{m}{2}\right]}\Big(t-\frac{1}{2}\Big) - t\Big)\Big)\\ &+2\Big(4k\Big(x^{\left[\frac{k}{2}\right]}\Big(t-\frac{1}{2}\Big) - t\Big)\Big(4m\Big(x^{\left[\frac{m}{2}\right]}\Big(t-\frac{1}{2}\Big) - t\Big)\Big)\\ &+m\Big(4k\Big(x^{\left[\frac{k}{2}\right]}\Big(t-\frac{1}{2}\Big) - t\Big) + 4(m-1)\Big(k\Big(x^{\left[\frac{k}{2}\right]}\Big(t-\frac{1}{2}\Big) - t\Big)\\ &+4k\Big(m\Big(x^{\left[\frac{m}{2}\right]}\Big(t-\frac{1}{2}\Big) - t\Big)\Big) + 4(k-1)\Big(m\Big(x^{\left[\frac{m}{2}\right]}\Big(t-\frac{1}{2}\Big) - t\Big)\Big).\end{aligned}$$

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Department of Mathematical Sciences,
Isfahan University of Technology,
Isfahan 84156-8311,
Iran
E–mail: eliasi@math.iut.ac.ir
b.taeri@cc.iut.ac.ir

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