

# Schultz polynomial and modified Schultz polynomial of a random benzenoid chain

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## Abstract

Let  $G$  be a graph with a vertex set  $V(G)$ ,  $d_G(u, v)$  and  $\delta_G(v)$  denote the topological distance between vertices  $u$  and  $v$  in  $G$  and the degree of the vertex  $v$  in  $G$ , respectively. The Schultz polynomial of  $G$  is defined as  $H^+(G) = \sum_{\{u,v\} \subseteq V(G)} (\delta_G(u) + \delta_G(v))x^{d_G(u,v)}$  and the modified Schultz polynomial of  $G$  is defined as  $H^*(G) = \sum_{\{u,v\} \subseteq V(G)} \delta_G(u)\delta_G(v)x^{d_G(u,v)}$ . In this paper, we obtain explicit analytical expressions for expected values of Schultz polynomial and modified Schultz polynomial of a random benzenoid chain with  $n$  hexagons. Further expected values of some related topological indices are obtained.

**Keywords:** Schultz polynomial, modified Schultz polynomial, random benzenoid chain, expected value, generating function.

## 1 Introduction

Let  $G$  be a graph with a vertex set  $V(G)$  and let  $d_G(u, v)$  denote the *topological distance* (or *distance* for short) between vertices  $u$  and  $v$  in  $G$ , i.e., the length of a shortest path connecting  $u$  and  $v$  in  $G$ ,  $\delta_G(u)$  denote the degree of vertex  $u$  in  $G$ , respectively. The subscript is omitted when there is no risk of confusion.

In 2005, I. Gutman introduced [3] two polynomials in variable  $x$  in  $G$ , called the *Schultz polynomial*  $H^+(G, x)$  and the *modified Schultz polynomial*

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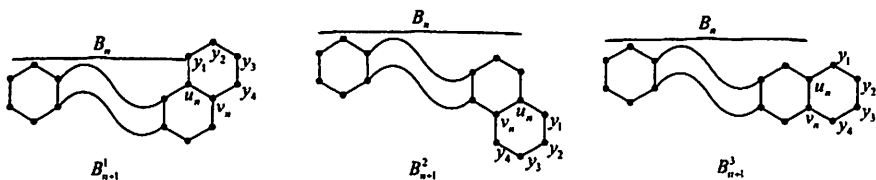


Fig. 1: The three types of local arrangements in benzenoid chains  $B_{n+1}$ .

$H^*(G, x)$ , which are analogs for the Hosoya polynomial  $H(G, x)$  introduced by Hosoya [2]. The definitions are as follows:

$$\begin{aligned}
 H^+(G, x) &= \sum_{\{u,v\} \subseteq V(G)} (\delta_G(u) + \delta_G(v)) x^{d_G(u,v)}, \\
 H^*(G, x) &= \sum_{\{u,v\} \subseteq V(G)} \delta_G(u) \delta_G(v) x^{d_G(u,v)}, \\
 H(G, x) &= \sum_{\{u,v\} \subseteq V(G)} x^{d_G(u,v)}.
 \end{aligned}$$

Here,  $u$  and  $v$  do not necessarily distinct. For some recently results about this field, we refer the readers to the Refs. [3, 5, 7, 8, 10].

Let  $B_{n+1}$  denote a benzenoid chain with  $n+1$  hexagons ( $n \geq 0$ ). There are obviously unique benzenoid chains  $B_{n+1}$  when  $n = 0, 1$ . More generally, a benzenoid chain  $B_{n+1}$  can be regarded as a benzenoid chain  $B_n$  to which a new terminal hexagon with vertices  $\{u_n, y_1, y_2, y_3, y_4, v_n\}$  is adjoined. However, when  $n \geq 2$ , the terminal hexagon can be attached in three ways, resulting in the local arrangements  $B_{n+1}^1, B_{n+1}^2, B_{n+1}^3$ , according to the related position of the terminal hexagon shown in Fig. 1.

A *random benzenoid chain*,  $R_{n+1}$  with  $n+1$  hexagons, is a benzenoid chain obtained by stepwise additions of terminal hexagons. As the initial steps,  $R_1 = B_1, R_2 = B_2$ , and for each step  $k$  ( $2 \leq k \leq n$ ) a random selection is made from one of the three possible constructions:

$$\begin{aligned}
 B_k &\rightarrow B_{k+1}^1, \text{ with probability } p_1, \\
 B_k &\rightarrow B_{k+1}^2, \text{ with probability } p_2 \text{ or} \\
 B_k &\rightarrow B_{k+1}^3, \text{ with probability } q = 1 - p_1 - p_2.
 \end{aligned}$$

We assume the probabilities  $p_1$  and  $p_2$  are constants, invariant to the step parameter  $k$ . That is, the process described is a Markov chain of order zero with a state space consisting of three states.

In the present paper, we calculate the expected value of the Schultz polynomial and modified Schultz polynomial of a random benzenoid chain  $R_n$  with  $n$  hexagons and give explicit analytical expressions by using the

combinatorial tool: generating function. Further, the expected values of some related topological indices are obtained.

## 2 Expected values of Schultz polynomials and modified Schultz polynomials

Let  $G$  be a connected graph with a vertex set  $V(G)$ . For the simplicity, we define a notation as follows: for a vertex  $u \in V(G)$ ,

$$H_G(u; x) = \sum_{v \in V(G)} x^{d(u,v)},$$

i.e., the contribution of the vertex  $u$  to the Hosoya polynomial  $H(G, x)$  of  $G$ . If we consider the effect of degree, we can define the other notation:

$$H_G^\delta(u; x) = \sum_{v \in V(G)} \delta(v) x^{d(u,v)}.$$

Hence, alternative formulae of  $H^+(G, x)$  and  $H^*(G, x)$  are expressed in terms of  $H_G^\delta(u; x)$  as

$$H^+(G, x) = \sum_{u \in V(G)} H_G^\delta(u; x) + \sum_{u \in V(G)} \delta(u), \quad (1)$$

$$H^*(G, x) = \frac{1}{2} \sum_{u \in V(G)} \delta(u) H_G^\delta(u; x) + \frac{1}{2} \sum_{u \in V(G)} \delta^2(u). \quad (2)$$

### 2.1 Recursion relations

As described in the previous section, a benzenoid chain  $B_{n+1}$  is obtained by attaching to a benzenoid chain  $B_n$  a terminal hexagon consisting of vertices  $u_n, y_1, y_2, y_3, y_4, v_n$  (see Fig. 1). Now, we will give some basic lemmas:

**Lemma 2.1.**

$$H_{B_{n+1}}(y_1; x) = xH_{B_n}(u_n; x) + x^3 + x^2 + x + 1, \quad (3a)$$

$$H_{B_{n+1}}(y_2; x) = x^2H_{B_n}(u_n; x) + x^2 + 2x + 1, \quad (3b)$$

$$H_{B_{n+1}}(y_3; x) = x^2H_{B_n}(v_n; x) + x^2 + 2x + 1, \quad (3c)$$

$$H_{B_{n+1}}(y_4; x) = xH_{B_n}(v_n; x) + x^3 + x^2 + x + 1. \quad (3d)$$

*Proof.* We only give the proofs of Eqs. (3a) and (3b). From the definition,

$$\begin{aligned} H_{B_{n+1}}(y_1; x) &= \sum_{w \in V(B_{n+1})} x^{d(y_1, w)} = \sum_{w \in V(B_n)} x^{d(u_n, w)+1} + x^3 + x^2 + x + 1 \\ &= x \sum_{w \in V(B_n)} x^{d(u_n, w)} + x^3 + x^2 + x + 1 = xH_{B_n}(u_n; x) + x^3 + x^2 + x + 1; \end{aligned}$$

$$\begin{aligned}
H_{B_{n+1}}(y_2; x) &= \sum_{w \in V(B_{n+1})} x^{d(y_2, w)} = \sum_{w \in V(B_n)} x^{d(u_n, w)+2} + x^2 + 2x + 1 \\
&= x^2 \sum_{w \in V(B_n)} x^{d(u_n, w)} + x^2 + 2x + 1 = x^2 H_{B_n}(u_n; x) + x^2 + 2x + 1.
\end{aligned}$$

We can prove Eqs. (3c) and (3d) in analogous ways.  $\square$

Similarly, we have

**Lemma 2.2.**

$$H_{B_{n+1}}^\delta(y_1; x) = xH_{B_n}^\delta(u_n; x) + 2x^3 + 3x^2 + 3x + 2, \quad (4a)$$

$$H_{B_{n+1}}^\delta(y_2; x) = x^2H_{B_n}^\delta(u_n; x) + x^3 + 3x^2 + 4x + 2, \quad (4b)$$

$$H_{B_{n+1}}^\delta(y_3; x) = x^2H_{B_n}^\delta(v_n; x) + x^3 + 3x^2 + 4x + 2, \quad (4c)$$

$$H_{B_{n+1}}^\delta(y_4; x) = xH_{B_n}^\delta(u_n; x) + 2x^3 + 3x^2 + 3x + 2, \quad (4d)$$

**Lemma 2.3.**

$$\begin{aligned}
H^+(B_{n+1}, x) &= H^+(B_n, x) + (x + x^2)(H_{B_n}^\delta(u_n; x) + H_{B_n}^\delta(v_n; x)) + \\
&(2x^2 + 2x + 1)(H_{B_n}(u_n; x) + H_{B_n}(v_n; x)) + 6x^3 + 12x^2 + 14x + 18. \quad (5)
\end{aligned}$$

$$\begin{aligned}
H^*(B_{n+1}, x) &= H^*(B_n, x) + (2x^2 + 2x + 1)(H_{B_n}^\delta(u_n; x) + H_{B_n}^\delta(v_n; x)) \\
&+ 8x^3 + 16x^2 + 17x + 22. \quad (6)
\end{aligned}$$

*Proof.* From the definition, applying Eqs. (3) and (4), we have

$$\begin{aligned}
H^+(B_{n+1}, x) &= \sum_{\{w, z\} \subseteq V(B_{n+1})} (\delta_{B_{n+1}}(w) + \delta_{B_{n+1}}(z))x^{d(w, z)} = \sum_{\{w, z\} \subseteq V(B_n)} \\
&(\delta_{B_{n+1}}(w) + \delta_{B_{n+1}}(z))x^{d(w, z)} + \sum_{\{w\} \subseteq V(B_{n+1}), \{z\} \subseteq \{y_1, y_2, y_3, y_4\}} (\delta_{B_{n+1}}(w) + \\
\delta_{B_{n+1}}(z))x^{d(w, z)} &= \left( \sum_{\{w, z\} \subseteq V(B_n) \setminus \{u_n, v_n\}} (\delta_{B_n}(w) + \delta_{B_n}(z))x^{d(w, z)} \right. \\
&+ \sum_{\{w\} \subseteq V(B_n) \setminus \{u_n, v_n\}, \{z\} \subseteq \{u_n, v_n\}} (\delta_{B_n}(w) + \delta_{B_n}(z) + 1)x^{d(w, z)} + \sum_{\{w, z\} \subseteq \{u_n, v_n\}} \\
&(\delta_{B_n}(w) + \delta_{B_n}(z) + 2)x^{d(w, z)} \left. \right) + \left( \sum_{\{w\} \subseteq V(B_{n+1}), \{z\} \subseteq \{y_1, y_2, y_3, y_4\}} \delta_{B_{n+1}}(w) \right. \\
&x^{d(w, z)} + \sum_{\{w\} \subseteq V(B_{n+1}), \{z\} \subseteq \{y_1, y_2, y_3, y_4\}} 2x^{d(w, z)} \left. \right) = \left( \sum_{\{w, z\} \subseteq V(B_n)} (\delta_{B_n}(w)
\end{aligned}$$

$$\begin{aligned}
& + \delta_{B_n}(z)x^{d(u,z)} + (H_{B_n}(u_n; x) + H_{B_n}(v_n; x) - 2(x+1)) + 2(x+2) \\
& + \left( \left( \sum_{i=1}^4 H_{B_{n+1}}^\delta(y_i; x) - 2(x^3 + 2x^2 + 3x) \right) + 2 \left( \sum_{i=1}^4 H_{B_{n+1}}(y_i; x) - (x^3 \right. \right. \\
& \left. \left. + 2x^2 + 3x) \right) \right) = H^+(B_n, x) + \sum_{i=1}^4 H_{B_{n+1}}^\delta(y_i; x) + 2 \sum_{i=1}^4 H_{B_{n+1}}(y_i; x) \\
& + H_{B_n}(u_n; x) + H_{B_n}(v_n; x) - 4x^3 - 8x^2 - 12x + 2 \\
& = H^+(B_n, x) + (x+x^2)(H_{B_n}^\delta(u_n; x) + H_{B_n}^\delta(v_n; x)) + (2x^2 + 2x + 1) \\
& \quad (H_{B_n}(u_n; x) + H_{B_n}(v_n; x)) + 6x^3 + 12x^2 + 14x + 18.
\end{aligned}$$

Similarly, we can prove Eq. (6).  $\square$

In fact, the equations discussed above associated with a specific benzenoid chain are valid for a random benzenoid chain, i.e., Eqs. (3)-(6) still hold when we simultaneously replace  $B_{n+1}$  for  $R_{n+1}$  and  $B_n$  for  $R_n$ .

In what following we consider contributions of  $u_{n+1}$  and  $v_{n+1}$  to  $H^+(B_{n+1}, x)$  and  $H^*(B_{n+1}, x)$  according to the positions of  $u_{n+1}$  and  $v_{n+1}$ . There are three cases to consider:

Case 1.  $B_{n+1} \rightarrow B_{n+2}^1$ . In this case,  $u_{n+1} = y_1$  and  $v_{n+1} = y_2$ . Consequently,  $H_{B_{n+1}}(u_{n+1}; x) = H_{B_{n+1}}(y_1; x)$  and  $H_{B_{n+1}}(v_{n+1}; x) = H_{B_{n+1}}(y_2; x)$ ,  $H_{B_{n+1}}^\delta(u_{n+1}; x) = H_{B_{n+1}}^\delta(y_1; x)$  and  $H_{B_{n+1}}^\delta(v_{n+1}; x) = H_{B_{n+1}}^\delta(y_2; x)$  which are given by Eqs. (3a) and (3b), Eqs. (4a) and (4b), respectively.

Case 2.  $B_{n+1} \rightarrow B_{n+2}^2$ . In this case,  $u_{n+1} = y_3$  and  $v_{n+1} = y_4$ . Consequently,  $H_{B_{n+1}}(u_{n+1}; x) = H_{B_{n+1}}(y_3; x)$  and  $H_{B_{n+1}}(v_{n+1}; x) = H_{B_{n+1}}(y_4; x)$ ,  $H_{B_{n+1}}^\delta(u_{n+1}; x) = H_{B_{n+1}}^\delta(y_3; x)$  and  $H_{B_{n+1}}^\delta(v_{n+1}; x) = H_{B_{n+1}}^\delta(y_4; x)$ , which are given by Eqs. (3c) and (3d), Eqs. (4c) and (4d), respectively.

Case 3.  $B_{n+1} \rightarrow B_{n+2}^3$ . In this case,  $u_{n+1} = y_2$  and  $v_{n+1} = y_3$ . Consequently,  $H_{B_{n+1}}(u_{n+1}; x) = H_{B_{n+1}}(y_2; x)$  and  $H_{B_{n+1}}(v_{n+1}; x) = H_{B_{n+1}}(y_3; x)$ ,  $H_{B_{n+1}}^\delta(u_{n+1}; x) = H_{B_{n+1}}^\delta(y_2; x)$  and  $H_{B_{n+1}}^\delta(v_{n+1}; x) = H_{B_{n+1}}^\delta(y_3; x)$ , which are given by Eqs. (3b) and (3c), Eqs. (4b) and (4c), respectively.

For a random benzenoid chain  $R_{n+1}$ ,  $H^+(R_{n+1}, x)$ ,  $H^*(R_{n+1}, x)$ ,  $H_{R_{n+1}}(u_{n+1}; x)$ ,  $H_{R_{n+1}}(v_{n+1}; x)$ ,  $H_{R_{n+1}}^\delta(u_{n+1}; x)$  and  $H_{R_{n+1}}^\delta(v_{n+1}; x)$  are random variables and we denote their expected values by  $H_{n+1}^+(x)$ ,  $H_{n+1}^*(x)$ ,  $U_{n+1}(x)$ ,  $V_{n+1}(x)$ ,  $U_{n+1}^\delta(x)$  and  $V_{n+1}^\delta(x)$ , respectively, i.e.,

$$\begin{aligned}
H_{n+1}^+(x) &= E(H^+(R_{n+1}, x)), H_{n+1}^*(x) = E(H^*(R_{n+1}, x)), \\
U_{n+1}(x) &= E(H_{R_{n+1}}(u_{n+1}; x)), V_{n+1}(x) = E(H_{R_{n+1}}(v_{n+1}; x)), \\
U_{n+1}^\delta(x) &= E(H_{R_{n+1}}^\delta(u_{n+1}; x)) \text{ and } V_{n+1}^\delta(x) = E(H_{R_{n+1}}^\delta(v_{n+1}; x)).
\end{aligned}$$

Since the above three cases occur in random benzenoid chains with probabilities  $p_1$ ,  $p_2$  and  $q = 1 - p_1 - p_2$ , respectively, by the definition of the

expected value we immediately obtain

$$U_{n+1}(x) = p_1 H_{R_{n+1}}(y_1; x) + p_2 H_{R_{n+1}}(y_3; x) + q H_{R_{n+1}}(y_2; x), \quad (7a)$$

$$V_{n+1}(x) = p_1 H_{R_{n+1}}(y_2; x) + p_2 H_{R_{n+1}}(y_4; x) + q H_{R_{n+1}}(y_3; x), \quad (7b)$$

$$U_{n+1}^\delta(x) = p_1 H_{R_{n+1}}^\delta(y_1; x) + p_2 H_{R_{n+1}}^\delta(y_3; x) + q H_{R_{n+1}}^\delta(y_2; x) \quad (7c)$$

$$V_{n+1}^\delta(x) = p_1 H_{R_{n+1}}^\delta(y_2; x) + p_2 H_{R_{n+1}}^\delta(y_4; x) + q H_{R_{n+1}}^\delta(y_3; x), \quad (7d)$$

Substituting the corresponding analogues associated with random benzenoid chains  $R_n$  and  $R_{n+1}$  to Eqs. (3) and (4) for Eq. (7), we get

$$U_{n+1}(x) = (p_1 x + q x^2) H_{R_n}(u_n; x) + p_2 x^2 H_{R_n}(v_n; x) + (x^3 - x)p_1 + (x + 1)^2,$$

$$V_{n+1}(x) = (p_2 x + q x^2) H_{R_n}(v_n; x) + p_1 x^2 H_{R_n}(u_n; x) + (x^3 - x)p_2 + (x + 1)^2,$$

$$U_{n+1}^\delta(x) = (p_1 x + q x^2) H_{R_n}^\delta(u_n; x) + p_2 x^2 H_{R_n}^\delta(v_n; x) + (1 + p_1)x^3 + 3x^2 + (4 - p_1)x + 2,$$

$$V_{n+1}^\delta(x) = (p_2 x + q x^2) H_{R_n}^\delta(v_n; x) + p_1 x^2 H_{R_n}^\delta(u_n; x) + (1 + p_2)x^3 + 3x^2 + (4 - p_2)x + 2.$$

By applying the expectation operator to the above equations, and noting that  $E(U_{n+1}(x)) = U_{n+1}(x)$ ,  $E(V_{n+1}(x)) = V_{n+1}(x)$ ,  $U_{n+1}^\delta(x) = E(H_{R_{n+1}}^\delta(u_{n+1}; x))$  and  $V_{n+1}^\delta(x) = E(H_{R_{n+1}}^\delta(v_{n+1}; x))$ . We obtain

$$U_{n+1}(x) = (p_1 x + q x^2) U_n(x) + p_2 x^2 V_n(x) + (x^3 - x)p_1 + (x + 1)^2, \quad (9a)$$

$$V_{n+1}(x) = (p_2 x + q x^2) V_n(x) + p_1 x^2 U_n(x) + (x^3 - x)p_2 + (x + 1)^2, \quad (9b)$$

$$U_{n+1}^\delta(x) = (p_1 x + q x^2) U_n^\delta(x) + p_2 x^2 V_n^\delta(x) + (1 + p_1)x^3 + 3x^2 + (4 - p_1)x + 2, \quad (9c)$$

$$V_{n+1}^\delta(x) = (p_2 x + q x^2) V_n^\delta(x) + p_1 x^2 U_n^\delta(x) + (1 + p_2)x^3 + 3x^2 + (4 - p_2)x + 2. \quad (9d)$$

A recursion relation for the expected value of the Schultz polynomials and modified Schultz polynomials of a random benzenoid chain can be obtained from Eqs. (5) and (6) by using  $R_k$  in place of  $B_k$  ( $k = n, n + 1$ ) and by using the expectation operator:

$$H_{n+1}^*(x) = H_n^*(x) + (2x^2 + 2x + 1)(U_n^\delta(x) + V_n^\delta(x)) + 8x^3 + 16x^2 + 17x + 22;$$

$$H_{n+1}^+(x) = H_n^+(x) + (x + x^2)(U_n^\delta(x) + V_n^\delta(x)) + (2x^2 + 2x + 1)(U_n(x) + V_n(x)) + 6x^3 + 12x^2 + 14x + 18. \quad (10)$$

In order to make the calculation more convenient, we assume that the system of recursion equations (9)-(10) holds for  $n \geq 0$ , and set boundary conditions as:

$$\begin{aligned} H_0^+(x) &= 2x + 4, H_0^*(x) = x, U_0(x) = x + 1, \\ V_0(x) &= x + 1, U_0^\delta(x) = x + 1, V_0^\delta(x) = x + 1. \end{aligned} \quad (11)$$

### 3 Solution for recursion equations

To solve the recursion equations (9)-(10), we use the method of the generating function [6]. We will use the fact that  $\sum_{n \geq 0} t^n = (1-t)^{-1}$ ,  $0 < t < 1$ ,

and define the following generating functions in variable  $t$ ,  $0 < t < 1$ :  
 $U(t) = \sum_{n \geq 0} U_n(x)t^n$ ,  $V(t) = \sum_{n \geq 0} V_n(x)t^n$ ,  $U^\delta(t) = \sum_{n \geq 0} U_n^\delta(x)t^n$ ,  $V^\delta(t) = \sum_{n \geq 0} V_n^\delta(x)t^n$ ,  $H^*(t) = \sum_{n \geq 0} H_n^*(x)t^n$  and  $H^+(t) = \sum_{n \geq 0} H_n^+(x)t^n$ .

From Eqs. (9)-(11), we get relations of their generating functions as follows:

$$U(t) = t(p_1x + qx^2)U(t) + p_2x^2tV(t) + \frac{t(x^3 - x)p_1 + t(x+1)^2}{1-t} + x + 1, \quad (12a)$$

$$V(t) = t(p_2x + qx^2)V(t) + p_1x^2tU(t) + \frac{t(x^3 - x)p_2 + t(x+1)^2}{1-t} + x + 1, \quad (12b)$$

$$U^\delta(t) = t(p_1x + qx^2)U^\delta(t) + p_2x^2tV^\delta(t) + \frac{t((1+p_1)x^3 + 3x^2 + (4-p_1)x + 2)}{1-t} + x + 1, \quad (12c)$$

$$V^\delta(t) = t(p_2x + qx^2)V^\delta(t) + p_1x^2tU^\delta(t) + \frac{t((1+p_2)x^3 + 3x^2 + (4-p_2)x + 2)}{1-t} + x + 1, \quad (12d)$$

$$H^+(t) = tH^+(t) + (x+x^2)t(U^\delta(t) + V^\delta(t)) + (1+2x+2x^2)t(U(t) + V(t)) + \frac{t(6x^3 + 12x^2 + 14x + 18)}{1-t} + 2x + 4, \quad (12e)$$

$$H^*(t) = tH^*(t) + (1+2x+2x^2)t(U^\delta(t) + V^\delta(t)) + \frac{t(8x^3 + 16x^2 + 17x + 22)}{1-t} + x. \quad (12f)$$

As Eqs. (12a) and (12b) form a system of two linear equations of variables  $U(t)$  and  $V(t)$ , a straightforward calculation yields:

$$U(t) = \frac{p_1x(x+1)^2}{(x-1)(1-xt)} + \frac{(1-p_1)x(x+1)}{(x-1)(1-x^2t)} + \frac{(p_1x^2+1)(x+1)}{(1-x)(1-t)} + \frac{p_2(p_1-p_2)t^2x^3(x+1)^2}{(1-t)(1-qt)} \left( \frac{1}{1-x^2t} - \frac{1}{1-xt} \right); \quad (13a)$$

$$V(t) = \frac{p_2x(x+1)^2}{(x-1)(1-xt)} + \frac{(1-p_2)x(x+1)}{(x-1)(1-x^2t)} + \frac{(p_2x^2+1)(x+1)}{(1-x)(1-t)} + \frac{p_1(p_2-p_1)t^2x^3(x+1)^2}{(1-t)(1-qt)} \left( \frac{1}{1-x^2t} - \frac{1}{1-xt} \right). \quad (13b)$$

As Eqs. (12c) and (12d) comprise a system of two linear equations in two variables  $U^d(t)$  and  $V^d(t)$ , a straight forward calculation results in

$$U^d(t) = \frac{p_1(2x^3 + 4x^2 + 3x + 1)}{(x-1)(1-xt)} + \frac{(1-p_1)(2x^2 + 2x + 1)}{(x-1)(1-x^2t)} + \frac{2p_1x^3 + (2p_1+1)x^2}{(1-x)(1-t)} \\ + \frac{(p_1+2)x+2}{(1-x)(1-t)} + \frac{p_2(p_1-p_2)t^2(x^3+x^2)(2x^2+2x+1)\left(\frac{1}{1-x^2t} - \frac{1}{1-xt}\right)}{(1-t)(1-qt)}; \quad (14a)$$

$$V^d(t) = \frac{p_2(2x^3 + 4x^2 + 3x + 1)}{(x-1)(1-xt)} + \frac{(1-p_2)(2x^2 + 2x + 1)}{(x-1)(1-x^2t)} + \frac{2p_2x^3 + (2p_2+1)x^2}{(1-x)(1-t)} \\ + \frac{(p_2+2)x+2}{(1-x)(1-t)} + \frac{p_1(p_2-p_1)t^2(x^3+x^2)(2x^2+2x+1)\left(\frac{1}{1-x^2t} - \frac{1}{1-xt}\right)}{(1-t)(1-qt)}. \quad (14b)$$

Substituting Eqs. (13) and (14) for Eq. (12e) and rearranging, we can once more easily get:

$$H^+(t) = \frac{2x+4}{1-t} + \frac{t(6x^3 + 12x^2 + 14x + 18)}{(1-t)^2} + \frac{t(1-q)2x(x+1)^2(2x^2+2x+1)}{(x-1)(1-t)(1-xt)} \\ + \frac{2t(1+x)(1+4x+(5-q)x^2+(3-2q)x^3+2(1-q)x^4)}{(1-t)^2(1-x)} + \frac{2x^3+4x^2+3x+1}{(x-1)} \\ - \frac{2xt(1+q)}{(1-t)(1-x^2t)} - \frac{(p_1-p_2)^2t^3(x+1)^2(4x^5+4x^4+2x^3)\left(\frac{1}{1-x^2t} - \frac{1}{1-xt}\right)}{(1-t)^2(1-qt)}. \quad (15)$$

Substituting Eqs. (13) and (14) for Eq. (12f) and rearranging, we can easily get:

$$H^*(t) = \frac{t(8x^3 + 16x^2 + 17x + 22)}{(1-t)^2} + \frac{t(1-q)(4x^5 + 12x^4 + 16x^3 + 12x^2 + 5x + 1)}{(x-1)(1-t)(1-xt)} \\ + \frac{x}{1-t} + \frac{t(4(1-q)x^5 + (12-8q)x^4 + (20-8q)x^3 + (22-4q)x^2 + (13-q)x + 4)}{(1-t)^2(1-x)} \\ + \frac{t(1+q)(2x^2+2x+1)^2}{(x-1)(1-t)(1-x^2t)} - \frac{(p_1-p_2)^2t^3(x^2+x^3)(1+2x+2x^2)\left(\frac{1}{1-x^2t} - \frac{1}{1-xt}\right)}{(1-t)^2(1-qt)}. \quad (16)$$

Applying Newton's generalized binomial theorem

$$(1-t)^{-j} = \sum_{n=0}^{+\infty} \binom{n+j-1}{j-1} t^n \quad (17)$$

to Eq. (15), and rearranging it, we get

$$H^+(t) = 2x+4 + 12(2+2x+2x^2+x^3)t + (44+50x+64x^2+52x^3+24x^4 \\ + 8x^5)t^2 + \sum_{n=3}^{+\infty} (2x+4 + \frac{(1-q)(x+1)^2(4x^3+4x^2+2x)(x^n-1)}{(x-1)^2} + (1+q)$$



$$\begin{aligned} & \frac{(4x^4 + 8x^3 + 6x^2 + 2x)(x^{2n} - 1)}{(x-1)^2(x+1)} + \frac{(4(1-q)x^5 + (4-8q)x^4 + (10-6q)x^3)n}{(1-x)} \\ & + \frac{2((8-q)x^2 + 3x + 10)n}{1-x} - (p_1 - p_2)^2(x+1)^2(4x^5 + 4x^4 + 2x^3) \sum_{l=0}^{n-3} q^l \left( \sum_{k=0}^{n-3-l} \right. \\ & \left. (n-l-k-2)(x^{2k} - x^k) \right) t^n. \end{aligned} \quad (18)$$

Applying Eq. (17) to Eq. (16) and rearranging it, we get

$$\begin{aligned} H^*(t) &= x + 12(2 + 2x + 2x^2 + x^3)t + (50 + 57x + 72x^2 + 56x^3 + 24x^4 + 8x^5)t^2 + \\ & \sum_{n=3}^{+\infty} \left( x + \frac{(1-q)(4x^5 + 12x^4 + 16x^3 + 12x^2 + 5x + 1)(x^n - 1)}{(x-1)^2} \right. \\ & + \frac{(4(1-q)x^5 + (4-8q)x^4 + (12-8q)x^3 + (21-4q)x^2 + (8-q)x + 26)n}{1-x} \\ & + \frac{(1+q)(2x^2 + 2x + 1)^2(x^{2n} - 1)}{(x-1)^2(x+1)} - (p_1 - p_2)^2(x^2 + x^3)(1 + 2x + 2x^2)^2 \sum_{l=0}^{n-3} q^l \\ & \left. \left( \sum_{k=0}^{n-3-l} (n-l-k-2)(x^{2k} - x^k) \right) \right) t^n. \end{aligned} \quad (19)$$

## 4 Results and Discussion

First, we give two main theorems of this paper. From Eq. (18), we have the following first main theorem.

**Theorem 4.1.** *Let  $H_n^+(x)$  be the expected value of the Schultz polynomial of a random benzenoid chain with  $n$  hexagons. Then*

$$H_1^+(x) = 12(2 + 2x + 2x^2 + x^3); H_2^+(x) = 44 + 50x + 64x^2 + 52x^3 + 24x^4 + 8x^5;$$

and when  $n \geq 3$ ,

$$\begin{aligned} H_n^+(x) &= 2x + 4 + \frac{(1-q)(x+1)^2(4x^3 + 4x^2 + 2x)(x^n - 1)}{(x-1)^2} \\ & + \frac{(1+q)(4x^4 + 8x^3 + 6x^2 + 2x)(x^{2n} - 1)}{(x-1)^2(x+1)} \\ & + \frac{(4(1-q)x^5 + (4-8q)x^4 + (10-6q)x^3 + 2(8-q)x^2 + 6x + 20)n}{(1-x)} - (p_1 - p_2)^2 \\ & (x+1)^2(4x^5 + 4x^4 + 2x^3) \sum_{l=0}^{n-3} q^l \sum_{k=0}^{n-3-l} (n-l-k-2)(x^{2k} - x^k). \end{aligned} \quad (20)$$

When  $q = 1$  (in this case  $p_1 = p_2 = 0$ ), a random benzenoid chain is definitely a linear benzenoid chain, i.e., a benzenoid chain without no turns. So from Theorem 4.1 we have

**Corollary 4.2.** [7, 8, 10] *Let  $G$  be a benzenoid chain with  $n$  hexagons. If  $G$  has no turns, then the Schultz polynomial of  $G$  is*

$$H^+(G, x) = \frac{2(2 - 5x - 4x^2 - 3x^3 + 2x^{1+2n} + 4x^{2+2n} + 4x^{3+2n})}{(x-1)^2} + \frac{2n(10 - 7x + 4x^2 - 5x^3 - 4x^4 + 2x^5)}{(x-1)^2}.$$

If  $p_1 = 1$  or  $p_2 = 1$ , a random benzenoid chain with  $n$  hexagons is definitely a helicene with  $n$  hexagons, then we get

**Corollary 4.3.** [7, 8, 10] *Let  $G$  be a helicene with  $n$  hexagons. Then the Schultz polynomial of  $G$  is*

$$H^+(G, x) = \frac{2(2 - 5x - 6x^2 - 8x^3 - 7x^6 + 2x^8 + x^n(x + 5x^2 + 11x^3 + 13x^4 + 8x^5))}{(x-1)^2} - \frac{18(x^4 + x^5)}{(x-1)^2} + \frac{4x^{n+6} + 2n(10 - 7x + 5x^2 - 3x^3 - 2x^4 + 2x^5 - x^6 - 2x^7 - 2x^8)}{(x-1)^2}.$$

Secondly, from Schultz polynomial, we can easily get Schultz index  $W^+(G)$  of a molecular graph  $G$  and it was introduced by Dobrynin and Kochetova [1] and Gutman [4], is equal to the first derivative of the Schultz polynomial in  $x = 1$ :

$$W^+(G) = \left. \frac{d}{dx} H^+(G, x) \right|_{x=1}. \quad (21)$$

And Klavzar and Gutman introduced modified Schultz index  $W^*(G)$  in literature [9], it is equal to the first derivative of the modified Schultz polynomial in  $x = 1$ :

$$W^*(G) = \left. \frac{d}{dx} H^*(G, x) \right|_{x=1}. \quad (22)$$

By Eqs. (20) and (21), we get its Schultz index,

**Corollary 4.4.** *Let  $W_n^+$  the expected value of the Schultz index of a random benzenoid chain with  $n$  hexagons. Then*

$$W_n^+ = 2 + 18n + 68n^2 + 20n^3 + \frac{20q(n^3 - 3n^2 + 2n)}{3} - \frac{20(p_1 - p_2)^2}{3} + \sum_{k=0}^{n-3} k(k+1)(k+2)q^{n-k-3}.$$

If  $q = 1$ , we can get the upper bound on  $W_n^+$ , i.e.,  $\frac{1}{3}(80n^3 + 144n^2 + 94n + 6)$ , which is also the Schultz index of the linear benzenoid chains (i.e., linear polyacenes); if  $p_1 = 1$  or  $p_2 = 1$ , hence  $q = 0$ , it is a helicene, whose Schultz index is  $\frac{1}{3}(40n^3 + 324n^2 - 166n + 126)$ .

From Eq. (19), we have the following second main theorem.

**Theorem 4.5.** *Let  $H_n^*$  the expected value of the modified Schultz polynomial of a random benzenoid chain with  $n$  hexagons. Then*

$$H_1^*(x) = 12(2 + 2x + 2x^2 + x^3); H_2^*(x) = 50 + 57x + 72x^2 + 56x^3 + 24x^4 + 8x^5;$$

and when  $n \geq 3$ ,

$$\begin{aligned} H_n^*(x) = & x + \frac{(1-q)(4x^5 + 12x^4 + 16x^3 + 12x^2 + 5x + 1)(x^n - 1)}{(x-1)^2} \\ & + \frac{(4(1-q)x^5 + (4-8q)x^4 + (12-8q)x^3 + (21-4q)x^2 + (8-q)x + 26)n}{1-x} \\ & + \frac{(1+q)(2x^2 + 2x + 1)^2(x^{2n} - 1)}{(x-1)^2(x+1)} - (p_1 - p_2)^2(x^2 + x^3)(1 + 2x + 2x^2)^2 \\ & \sum_{l=0}^{n-3} q^l \sum_{k=0}^{n-3-l} (n-l-k-2)(x^{2k} - x^k). \end{aligned} \quad (23)$$

When  $q = 1$  (in this case  $p_1 = p_2 = 0$ ), a random benzenoid chain is definitely a linear benzenoid chain, i.e., a benzenoid chain without no turns. So from Theorem 4.5 we have

**Corollary 4.6.** [7, 8, 10] *Let  $G$  be a benzenoid chain with  $n$  hexagons. If  $G$  has no turns, then modified Schultz polynomial of  $G$  is*

$$\begin{aligned} H^*(G, x) = & x + n(22 + 17x + 16x^2 + 8x^3) - \frac{2n(2 + 6x + 9x^2 + 6x^3 + 2x^4)}{x-1} \\ & + \frac{2(1 + 2x + 2x^2)^2(x^{2n} - 1)}{(x-1)^2(1+x)}. \end{aligned}$$

If  $p_1 = 1$  or  $p_2 = 1$ , a random benzenoid chain with  $n$  hexagons is definitely a helicene with  $n$  hexagons, then we get

**Corollary 4.7.** [7, 8, 10] *Let  $G$  be a helicene with  $n$  hexagons. Then the modified Schultz polynomial of  $G$  is*

$$\begin{aligned} H^*(G, x) = & \frac{x^n(4x^6 + 16x^5 + 28x^4 + 28x^3 + 17x^2 + 6x + 1) + 4x^8 - 12x^6 - 20x^5 - 23x^4}{(x-1)^2} \\ & - \frac{21x^3 + 19x^2 + 7x + 2 + n(4x^8 + 4x^7 + 4x^6 - 4x^5 + 5x^4 + 8x^3 - 13x^2 + 18x - 26)}{(x-1)^2}. \end{aligned}$$

By Eqs. (22) and (23), we get its modified Schultz index,

**Corollary 4.8.** *Let  $W_n^*$  the expected value of the modified Schultz index of a random benzenoid chain with  $n$  hexagons. Then*

$$W_n^* = 1 + 12n + 70n^2 + 25n^3 + \frac{25q(n^3 - 3n^2 + 2n)}{3} - \frac{25(p_1 - p_2)^2}{3} \\ \sum_{k=0}^{n-3} k(k+1)(k+2)q^{n-k-3}.$$

If  $q = 1$ , we can get the upper bound  $\frac{1}{3}(100n^3 + 135n^2 + 86n + 3)$  on  $W_n^*$ , which is also the modified Schultz index of the linear benzenoid chain; if  $p_1 = 1$  or  $p_2 = 1$ , hence  $q = 0$ , it is a helicene, we can get its modified Schultz index:  $\frac{1}{3}(50n^3 + 360n^2 - 239n + 153)$ .

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