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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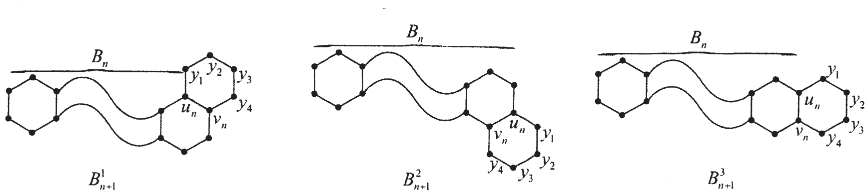

Fig. 1: The three types of local arrangements in benzenoid chains B_{n+1}.

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

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

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 ($n \geqslant 0$). 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 $n \geqslant 2$, the terminal hexagon can be attached in three ways, resulting in the local arrangements B^1_{n+1}, B^2_{n+1}, B^3_{n+1}, 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 ($2 \leqslant k \leqslant n$) a random selection is made from one of the three possible constructions:

$B_k \to B^1_{k+1}$, with probability p_1,
$B_k \to B^2_{k+1}$, with probability p_2 or
$B_k \to B^3_{k+1}$, with probability $q = 1 - p_1 - p_2$.

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

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

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

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.

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

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

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

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

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

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

$$= x\sum_{w\in V(B_n)} x^{d(u_n,w)} + x^3 + x^2 + x + 1 = xH_{B_n}(u_n;x) + x^3 + x^2 + x + 1;$$

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

We can prove Eqs. (3c) and (3d) in analogous ways. □

Similarly, we have

Lemma 2.2.

$$H^{\delta}_{B_{n+1}}(y_1;x) = xH^{\delta}_{B_n}(u_n;x) + 2x^3 + 3x^2 + 3x + 2, \tag{4a}$$
$$H^{\delta}_{B_{n+1}}(y_2;x) = x^2H^{\delta}_{B_n}(u_n;x) + x^3 + 3x^2 + 4x + 2, \tag{4b}$$
$$H^{\delta}_{B_{n+1}}(y_3;x) = x^2H^{\delta}_{B_n}(v_n;x) + x^3 + 3x^2 + 4x + 2, \tag{4c}$$
$$H^{\delta}_{B_{n+1}}(y_4;x) = xH^{\delta}_{B_n}(u_n;x) + 2x^3 + 3x^2 + 3x + 2, \tag{4d}$$

Lemma 2.3.

$$H^{+}(B_{n+1},x) = H^{+}(B_n,x) + (x+x^2)(H^{\delta}_{B_n}(u_n;x) + H^{\delta}_{B_n}(v_n;x)) + (2x^2+2x+1)(H_{B_n}(u_n;x) + H_{B_n}(v_n;x)) + 6x^3 + 12x^2 + 14x + 18. \tag{5}$$
$$H^{*}(B_{n+1},x) = H^{*}(B_n,x) + (2x^2+2x+1)(H^{\delta}_{B_n}(u_n;x) + H^{\delta}_{B_n}(v_n;x)) + 8x^3 + 16x^2 + 17x + 22. \tag{6}$$

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

$$H^{+}(B_{n+1},x) = \sum_{\{w,z\}\subseteq V(B_{n+1})} (\delta_{B_{n+1}}(w) + \delta_{B_{n+1}}(z))x^{d(w,z)} = \sum_{\{w,z\}\subseteq V(B_n)} (\delta_{B_{n+1}}(w) + \delta_{B_{n+1}}(z))x^{d(w,z)} + \sum_{\{w\}\subseteq V(B_{n+1}),\{z\}\subseteq\{y_1,y_2,y_3,y_4\}} (\delta_{B_{n+1}}(w) + \delta_{B_{n+1}}(z))x^{d(w,z)} = \Big(\sum_{\{w,z\}\subseteq V(B_n)\setminus\{u_n,v_n\}} (\delta_{B_n}(w) + \delta_{B_n}(z))x^{d(w,z)}$$
$$+ \sum_{\{w\}\subseteq V(B_n)\setminus\{u_n,v_n\},\{z\}\subseteq\{u_n,v_n\}} (\delta_{B_n}(w)+\delta_{B_n}(z)+1)x^{d(w,z)} + \sum_{\{w,z\}\subseteq\{u_n,v_n\}} (\delta_{B_n}(w) + \delta_{B_n}(z) + 2)x^{d(w,z)}\Big) + \Big(\sum_{\{w\}\subseteq V(B_{n+1}),\{z\}\subseteq\{y_1,y_2,y_3,y_4\}} \delta_{B_{n+1}}(w) x^{d(w,z)} + \sum_{\{w\}\subseteq V(B_{n+1}),\{z\}\subseteq\{y_1,y_2,y_3,y_4\}} 2x^{d(w,z)}\Big) = \Big(\sum_{\{w,z\}\subseteq V(B_n)} (\delta_{B_n}(w)$$

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

Similarly, we can prove Eq. (6). □

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. $B_{n+1}\to B^{1}_{n+2}$. 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 $H_{B_{n+1}}(v_{n+1};x)=H_{B_{n+1}}(y_2;x)$, $H^{\delta}_{B_{n+1}}(u_{n+1};x)=H^{\delta}_{B_{n+1}}(y_1;x)$ and $H^{\delta}_{B_{n+1}}(v_{n+1};x)=H^{\delta}_{B_{n+1}}(y_2;x)$ which are given by Eqs. (3a) and (3b), Eqs. (4a) and (4b), respectively.

Case 2. $B_{n+1}\to B^{2}_{n+2}$. 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 $H_{B_{n+1}}(v_{n+1};x)=H_{B_{n+1}}(y_4;x)$, $H^{\delta}_{B_{n+1}}(u_{n+1};x)=H^{\delta}_{B_{n+1}}(y_3;x)$ and $H^{\delta}_{B_{n+1}}(v_{n+1};x)=H^{\delta}_{B_{n+1}}(y_4;x)$, which are given by Eqs. (3c) and (3d), Eqs. (4c) and (4d), respectively.

Case 3. $B_{n+1}\to B^{3}_{n+2}$. 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 $H_{B_{n+1}}(v_{n+1};x)=H_{B_{n+1}}(y_3;x)$, $H^{\delta}_{B_{n+1}}(u_{n+1};x)=H^{\delta}_{B_{n+1}}(y_2;x)$ and $H^{\delta}_{B_{n+1}}(v_{n+1};x)=H^{\delta}_{B_{n+1}}(y_3;x)$, which are given by Eqs. (3b) and (3c), Eqs. (4b) and (4c), respectively.

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

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

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

$$U_{n+1}(x) = p_1 H_{R_{n+1}}(y_1; x) + p_2 H_{R_{n+1}}(y_3; x) + q H_{R_{n+1}}(y_2; x), \quad (7a)$$
$$V_{n+1}(x) = p_1 H_{R_{n+1}}(y_2; x) + p_2 H_{R_{n+1}}(y_4; x) + q H_{R_{n+1}}(y_3; x), \quad (7b)$$
$$U^{\delta}_{n+1}(x) = p_1 H^{\delta}_{R_{n+1}}(y_1; x) + p_2 H^{\delta}_{R_{n+1}}(y_3; x) + q H^{\delta}_{R_{n+1}}(y_2; x) \quad (7c)$$
$$V^{\delta}_{n+1}(x) = p_1 H^{\delta}_{R_{n+1}}(y_2; x) + p_2 H^{\delta}_{R_{n+1}}(y_4; x) + q H^{\delta}_{B_{n+1}}(y_3; x), \quad (7d)$$

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

$$U_{n+1}(x) = (p_1 x + qx^2) H_{R_n}(u_n; x) + p_2 x^2 H_{R_n}(v_n; x) + (x^3 - x)p_1 + (x+1)^2,$$
$$V_{n+1}(x) = (p_2 x + qx^2) H_{R_n}(v_n; x) + p_1 x^2 H_{R_n}(u_n; x) + (x^3 - x)p_2 + (x+1)^2,$$
$$U^{\delta}_{n+1}(x) = (p_1 x + qx^2) H^{\delta}_{R_n}(u_n; x) + p_2 x^2 H^{\delta}_{R_n}(v_n; x) + (1+p_1)x^3 + 3x^2 + (4-p_1)x + 2,$$
$$V^{\delta}_{n+1}(x) = (p_2 x + qx^2) H^{\delta}_{R_n}(v_n; x) + p_1 x^2 H^{\delta}_{R_n}(u_n; x) + (1+p_2)x^3 + 3x^2 + (4-p_2)x + 2.$$

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

$$U_{n+1}(x) = (p_1 x + qx^2)U_n(x) + p_2 x^2 V_n(x) + (x^3 - x)p_1 + (x+1)^2, \quad (9a)$$
$$V_{n+1}(x) = (p_2 x + qx^2)V_n(x) + p_1 x^2 U_n(x) + (x^3 - x)p_2 + (x+1)^2, \quad (9b)$$
$$U^{\delta}_{n+1}(x) = (p_1 x + qx^2)U^{\delta}_n(x) + p_2 x^2 V^{\delta}_n(x) + (1+p_1)x^3 + 3x^2 + (4-p_1)x + 2, \quad (9c)$$
$$V^{\delta}_{n+1}(x) = (p_2 x + qx^2)V^{\delta}_n(x) + p_1 x^2 U^{\delta}_n(x) + (1+p_2)x^3 + 3x^2 + (4-p_2)x + 2. \quad (9d)$$

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:

$$H^*_{n+1}(x) = H^*_n(x) + (2x^2 + 2x + 1)(U^{\delta}_n(x) + V^{\delta}_n(x)) + 8x^3 + 16x^2 + 17x + 22;$$
$$H^+_{n+1}(x) = H^+_n(x) + (x + x^2)(U^{\delta}_n(x) + V^{\delta}_n(x)) + (2x^2 + 2x + 1)(U_n(x) + V_n(x)) + 6x^3 + 12x^2 + 14x + 18. \quad (10)$$

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

$$H^+_0(x) = 2x + 4, H^*_0(x) = x, U_0(x) = x + 1,$$
$$V_0(x) = x + 1, U^{\delta}_0(x) = x + 1, V^{\delta}_0(x) = x + 1. \quad (11)$$

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

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

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

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

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:

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

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

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

$$\frac{(4x^4+8x^3+6x^2+2x)(x^{2n}-1)}{(x-1)^2(x+1)} + \frac{(4(1-q)x^5+(4-8q)x^4+(10-6q)x^3)n}{(1-x)}$$
$$+ \frac{2((8-q)x^2+3x+10)n}{1-x} - (p_1-p_2)^2(x+1)^2(4x^5+4x^4+2x^3)\sum_{l=0}^{n-3} q^l (\sum_{k=0}^{n-3-l}$$
$$(n-l-k-2)(x^{2k}-x^k)))t^n. \tag{18}$$

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

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

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 $n \geqslant 3$,

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

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 $x = 1$:

$$W^+(G) = \frac{\mathrm{d}}{\mathrm{d}x} H^+(G,x)\bigg|_{x=1}. \tag{21}$$

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 $x = 1$:

$$W^*(G) = \frac{\mathrm{d}}{\mathrm{d}x} H^*(G,x)\bigg|_{x=1}. \tag{22}$$

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 polyacences); 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 $n \geqslant 3$,

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

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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