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Research Article

Merrifield-Simmons Index in Random Phenylene Chains and Random Hexagon Chains

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The author obtains explicit expressions for the expected value of the Merrifield-Simmons index of a random phenylene chain and a random hexagon chain, respectively. The author also computes the corresponding entropy constants and obtains the maximum and minimum values in both random systems, respectively.

1. Introduction

Let $G = (V, E)$ be a simple undirected graph on n vertices. Two vertices of G are said to be independent if they are not adjacent in G. A k-independent set of G is a set of k mutually independent vertices. Denote by $i(G, k)$ the number of the k-independent sets of G. By definition, the empty vertex set is an independent set. Then $i(G, 0) = 1$ for any graph G. The Merrifield-Simmons index of G, denoted by $i(G)$, is defined as $i(G) = \sum_{k=0}^{n} i(G, k)$. So $i(G)$ is equal to the total number of the independent sets of G. The Merrifield-Simmons index was introduced in 1982 by Prodinger and Tichy [1], where it was called the Fibonacci number of a graph. The Merrifield-Simmons index is one of the most popular topological indices in chemistry intensively studied, as seen in the monograph [2]. Recently, there have been many papers studying the Merrifield-Simmons index for a graph. For more details see [3–8], among others.

Phenylenes are a class of conjugated hydrocarbons composed of six- and four-membered rings, where the six-membered rings (hexagons) are adjacent only to four-membered rings, and every four-membered ring is adjacent to a pair of nonadjacent hexagons. If each six-membered ring of a phenylene is adjacent only to two four-membered rings, we say that is a phenylene chain. Due to their aromatic and antiaromatic rings, phenylenes exhibit unique physicochemical properties. In Figure 1, some examples of phenylene chains are presented. The unique phenylene chains for $n = 1$ and $n = 2$ are shown in Figure 1. More generally, a phenylene chain with $n + 1$ hexagons (see Figure 2) can be regarded as a phenylene chain PH_n, with n hexagons to which a new terminal hexagon has been adjoined by a four-membered ring. But, for $n \geq 3$, the terminal hexagon can be attached in three ways, which results in the local arrangements we describe as PH_{n+1}^1, PH_{n+1}^2, and PH_{n+1}^3 (see Figure 3). Naturally, we define a random phenylene chain $\mathrm{PH}(n, p)$ with n hexagons as a phenylene chain obtained by stepwise addition of terminal hexagons. At each step k $(=3, 4, \ldots, n)$ a random selection is made from one of the three possible constructions: (1) $\mathrm{PH}_{k-1} \to \mathrm{PH}_k^1$, with probability p, (2) $\mathrm{PH}_{k-1} \to \mathrm{PH}_k^2$, with probability p, or (3) $\mathrm{PH}_{k-1} \to \mathrm{PH}_k^3$, with probability $q = 1 - 2p$.

We assume that the probability p is a constant, invariant to the step parameter k. That is, the process described is a zeroth-order Markov process.

By eliminating, "squeezing out," the squares from a phenylene, a catacondensed hexagonal system (which may be jammed) is obtained, called the hexagonal squeeze of the respective phenylene (see Figure 4). Clearly, there is a one-to-one correspondence between a phenylene (PH) and its hexagonal squeeze (HS). Both possess the same number of hexagons. The respective hexagonal squeeze of a random phenylene chain $\mathrm{PH}_{n,p}$ is a random hexagonal chain, and we denote it by $\mathrm{HS}_{n,p}$.

The Wiener index and the number of perfect matchings of a random hexagonal chain $\mathrm{HS}_{n,p}$ have been studied

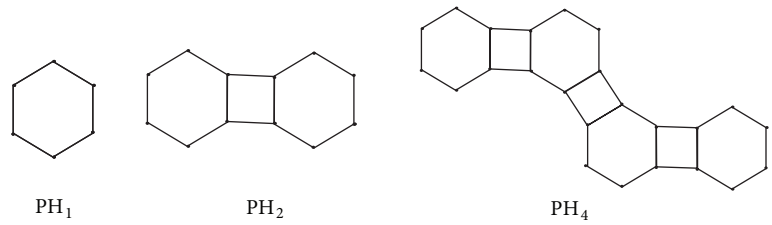

Figure 1: Phenylene chains.

by Gutman et al. [8–10]. Analogous results for a random phenylene chain $\mathrm{PH}_{n,p}$ have been obtained by Chen and Zhang in [11]. In this paper we obtain explicit expressions for the expected value of the Merrifield-Simmons index of a random phenylene chain $\mathrm{PH}_{n,p}$ and a random hexagonal chain $\mathrm{HS}_{n,p}$, respectively. We also compute the corresponding entropy constants and obtain the maximum and minimum values in both random systems, respectively. For some recent results on these hexagonal structures, see [12, 13].

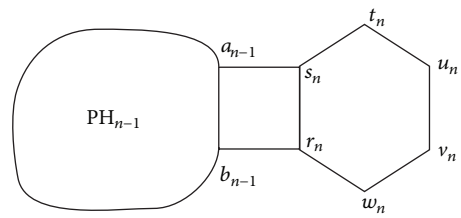

Figure 2: PH_n.

2. Merrifield-Simmons Index of a Random Phenylene Chain

Firstly, let us recall some results in [14], useful to this paper.

Lemma 1 (see [14]). *Consider $i(G_1 \cup G_2) = i(G_1)i(G_2)$.*

Lemma 2 (see [14]). *Let u be a vertex of G and let N_u be the subset of $V(G)$ consisting of the vertex u and its neighbors. Then*

$$i(G) = i(G-u) + i(G-N_u). \tag{1}$$

As described above, the phenylene chain PH_n can be obtained by adjoining to PH_{n-1} a hexagon by a 4-membered ring. For this construction, the following relations are easily obtained by Lemmas 1 and 2.

Lemma 3. *Let PH_n be denoted as a phenylene chain as in Figure 2; then for $n \geq 2$ one has*

$$\begin{aligned} i(PH_n) &= 8i(PH_{n-1}) \\ &\quad + 5\left[i(PH_{n-1}-a_{n-1}) + i(PH_{n-1}-b_{n-1})\right], \\ i(PH_n - a) &= \begin{cases} 5i(PH_{n-1}) + 5i(PH_{n-1}-a_{n-1}) \\ \quad +3i(PH_{n-1}-b_{n-1}), & \text{if } a = t_n, \\ 6i(PH_{n-1}) + 3i(PH_{n-1}-a_{n-1}) \\ \quad +4i(PH_{n-1}-b_{n-1}), & \text{if } a = u_n, \\ 6i(PH_{n-1}) + 4i(PH_{n-1}-a_{n-1}) \\ \quad +3i(PH_{n-1}-b_{n-1}), & \text{if } a = v_n, \\ 5i(PH_{n-1}) + 3i(PH_{n-1}-a_{n-1}) \\ \quad +5i(PH_{n-1}-b_{n-1}), & \text{if } a = w_n. \end{cases} \end{aligned} \tag{2}$$

Proof. Consider

$$\begin{aligned} i(\mathrm{PH}_n) &= i(\mathrm{PH}_n - s_n) + i((\mathrm{PH}_{n-1} - a_{n-1}) \cup P_3) \\ &= i(\mathrm{PH}_{n-1} \cup P_4) + i((\mathrm{PH}_{n-1} - b_{n-1}) \cup P_3) \\ &\quad + i((\mathrm{PH}_{n-1} - a_{n-1}) \cup P_3) \\ &= i(P_4)\, i(\mathrm{PH}_{n-1}) \\ &\quad + i(P_3)\left[i(\mathrm{PH}_{n-1} - b_{n-1}) + i(\mathrm{PH}_{n-1} - a_{n-1})\right] \\ &= 8i(\mathrm{PH}_{n-1}) \\ &\quad + 5\left[i(\mathrm{PH}_{n-1} - a_{n-1}) + i(\mathrm{PH}_{n-1} - b_{n-1})\right], \\ i(\mathrm{PH}_n - t_n) &= i(\mathrm{PH}_n - t_n - s_n) + i((\mathrm{PH}_{n-1} - a_{n-1}) \cup P_3) \\ &= i(\mathrm{PH}_{n-1} \cup P_3) + i((\mathrm{PH}_{n-1} - b_{n-1}) \cup P_2) \\ &\quad + i((\mathrm{PH}_{n-1} - a_{n-1}) \cup P_3) \\ &= i(P_3)\, i(\mathrm{PH}_{n-1}) + i(P_2)\, i(\mathrm{PH}_{n-1} - b_{n-1}) \\ &\quad + i(P_3)\, i(\mathrm{PH}_{n-1} - a_{n-1}) \\ &= 5i(\mathrm{PH}_{n-1}) + 5i(\mathrm{PH}_{n-1} - a_{n-1}) \\ &\quad + 3i(\mathrm{PH}_{n-1} - b_{n-1}), \\ i(\mathrm{PH}_n - u_n) &= i((\mathrm{PH}_n - u_n - s_n)) + i((\mathrm{PH}_{n-1} - a_{n-1}) \cup P_2) \\ &= i(\mathrm{PH}_{n-1} \cup P_1 \cup P_2) + i((\mathrm{PH}_{n-1} - b_{n-1}) \cup 2P_1) \\ &\quad + i((\mathrm{PH}_{n-1} - a_{n-1}) \cup P_2) \\ &= i(P_1)\, i(P_2)\, i(\mathrm{PH}_{n-1}) + i^2(P_1)\, i(\mathrm{PH}_{n-1} - b_{n-1}) \end{aligned}$$

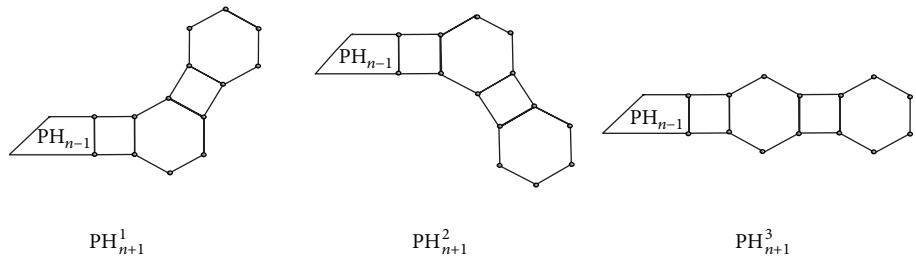

Figure 3: The three types of local arrangements in phenylene chains.

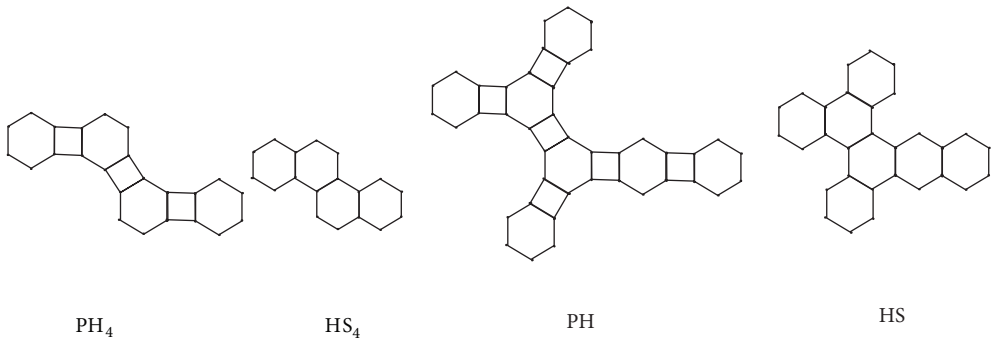

Figure 4: Phenylenes and the corresponding hexagonal squeezes.

$$\begin{aligned} &+ i(P_2)\, i(\mathrm{PH}_{n-1} - a_{n-1}) \\ &= 6i(\mathrm{PH}_{n-1}) + 3i(\mathrm{PH}_n - a_{n-1}) \\ &\quad + 4i(\mathrm{PH}_{n-1} - b_{n-1}). \end{aligned} \tag{3}$$

By the symmetry,

$$\begin{aligned} i(\mathrm{PH}_n - v_n) &= 6i(\mathrm{PH}_{n-1}) + 4i(\mathrm{PH}_{n-1} - a_{n-1}) \\ &\quad + 3i(\mathrm{PH}_n - b_{n-1}), \\ i(\mathrm{PH}_n - w_n) &= 5i(\mathrm{PH}_{n-1}) + 3i(\mathrm{PH}_{n-1} - a_{n-1}) \\ &\quad + 5i(\mathrm{PH}_{n-1} - b_{n-1}). \end{aligned} \tag{4}$$

For a random phenylene chain $\mathrm{PH}_{n,p}$, the Merrifield-Simmons indices $i(\mathrm{PH}_{n,p})$, $i(\mathrm{PH}_{n,p} - a_n)$, and $i(\mathrm{PH}_{n,p} - b_n)$ are random variables and we denote their expected values by $I_n = E[i(\mathrm{PH}_{n,p})]$, $U_n = E[i(\mathrm{PH}_{n,p} - a_n)]$, and $V_n = E[i(\mathrm{PH}_{n,p} - b_n)]$, respectively.

By the definition of $\mathrm{PH}_{n,p}$, we immediately have that, for $n \geq 2$,

$$\begin{aligned} I_n &= 8I_{n-1} + 5[U_{n-1} + V_{n-1}], \\ U_n &= pE\left[5i\left(\mathrm{PH}_{n-1,p}\right) + 5i\left(\mathrm{PH}_{n-1,p} - a_{n-1}\right)\right. \\ &\quad \left. + 3i\left(\mathrm{PH}_{n-1,p} - b_{n-1}\right)\right] \\ &\quad + pE\left[6i\left(\mathrm{PH}_{n-1,p}\right) + 4i\left(\mathrm{PH}_{n-1,p} - a_{n-1}\right)\right. \\ &\quad \left. + 3i\left(\mathrm{PH}_{n-1,p} - b_{n-1}\right)\right] \\ &\quad + (1-2p)E\left[6i\left(\mathrm{PH}_{n-1,p}\right) + 3i\left(\mathrm{PH}_{n-1,p} - a_{n-1}\right)\right. \\ &\quad \left. + 4i\left(\mathrm{PH}_{n-1,p} - b_{n-1}\right)\right] \\ &= (6-p)E\left[i\left(\mathrm{PH}_{n-1,p}\right)\right] \\ &\quad + (3+3p)E\left[i\left(\mathrm{PH}_{n-1,p} - a_{n-1}\right)\right] \\ &\quad + (4-2p)E\left[i\left(\mathrm{PH}_{n-1,p} - b_{n-1}\right)\right] \\ &= (6-p)I_{n-1} + (3+3p)U_{n-1} + (4-2p)V_{n-1}. \end{aligned} \tag{5}$$

By the symmetry,

$$V_n = (6-p)I_{n-1} + (4-2p)U_{n-1} + (3+3p)V_{n-1}. \tag{6}$$

To solve the recursion equation, we use the method of the generating functions. Set

$$I(t) = \sum_{n\geq 1} I_n t^n, \qquad U(t) = \sum_{n\geq 1} U_n t^n, \qquad V(t) = \sum_{n\geq 1} V_n t^n. \tag{7}$$

Then we have that

$$\begin{aligned} I(t) - 18t &= 8tI(t) + 5t[U(t) + V(t)], \\ U(t) - 13t &= (6-p)tI(t) + (4-2p)tV(t) \\ &\quad + (3+3p)tU(t), \end{aligned}$$

$$V(t) - 13t = (6-p)\,tI(t) + (3+3p)\,tV(t) + (4-2p)\,tU(t). \tag{8}$$

Recall that $I_1 = 18$, $I_2 = 274$, and $U_1 = V_1 = 13$.

Solving the equations, we have that

$$\begin{aligned} I(t) &= \frac{2t(9+2t-9pt)}{1-15t-pt-4t^2+18pt^2} \\ &= \frac{At}{1-\left(\left(15+p+\sqrt{241-42p+p^2}\right)/2\right)t} \\ &\quad + \frac{Bt}{1-\left(\left(15+p-\sqrt{241-42p+p^2}\right)/2\right)t}, \end{aligned} \tag{9}$$

where

$$\begin{aligned} A &= 9 + \frac{(139-9p)\sqrt{241-42p+p^2}}{241-42p+p^2}, \\ B &= 9 - \frac{(139-9p)\sqrt{241-42p+p^2}}{241-42p+p^2}. \end{aligned} \tag{10}$$

□

So we have the following result.

Theorem 4. *If $0 \le p \le 1/2$, then for $n \ge 2$ one has that*

$$E\left[i\left(PH_{n,p}\right)\right] = A\left(\frac{15+p+\sqrt{241-42p+p^2}}{2}\right)^{n-1} + B\left(\frac{15+p-\sqrt{241-42p+p^2}}{2}\right)^{n-1}, \tag{11}$$

where

$$\begin{aligned} A &= 9 + \frac{(139-9p)\sqrt{241-42p+p^2}}{241-42p+p^2}, \\ B &= 9 - \frac{(139-9p)\sqrt{241-42p+p^2}}{241-42p+p^2}. \end{aligned} \tag{12}$$

Specifically, one has that

$$\begin{aligned} E\left[i\left(PH_{n,1/2}\right)\right] &= \left(9+\frac{269\sqrt{881}}{881}\right)\left(\frac{31+\sqrt{881}}{4}\right)^{n-1} + \left(9-\frac{269\sqrt{881}}{881}\right)\left(\frac{31-\sqrt{881}}{4}\right)^{n-1}, \\ E\left[i\left(PH_{n,1/3}\right)\right] &= \left(9+\frac{204\sqrt{511}}{511}\right)\left(\frac{23+\sqrt{511}}{3}\right)^{n-1} + \left(9-\frac{204\sqrt{511}}{511}\right)\left(\frac{23-\sqrt{511}}{3}\right)^{n-1}, \\ E\left[i\left(PH_{n,0}\right)\right] &= \left(9+\frac{139\sqrt{241}}{241}\right)\left(\frac{15+\sqrt{241}}{2}\right)^{n-1} + \left(9-\frac{139\sqrt{241}}{241}\right)\left(\frac{15-\sqrt{241}}{2}\right)^{n-1}. \end{aligned} \tag{13}$$

The following corollary is easily obtained from Theorem 4 which gives the limits of the entropy constant $\log E[i(\mathrm{PH}_{n,p})]/|V(\mathrm{PH}_{n,p})|$ as $n \to +\infty$, where $V(\mathrm{PH}_{n,p})$ is the vertex set of $\mathrm{PH}_{n,p}$.

Corollary 5. *If $0 \le p \le 1/2$, then for $n \ge 2$, one has*

$$\begin{aligned} &\lim_{n\to+\infty} \frac{\log E\left[i\left(PH_{n,p}\right)\right]}{\left|V\left(PH_{n,p}\right)\right|} \\ &= \lim_{n\to+\infty} \frac{\log E\left[i\left(PH_{n,p}\right)\right]}{6n} \\ &= \frac{15+p+\sqrt{241-42p+p^2}}{12}. \end{aligned} \tag{14}$$

It is easy to check that $f(p) = (15+p+\sqrt{241-42p+p^2})/12$ is a monotonic decreasing function on p, so the limit of $\log E[i(PH_{n,p})]/6n$ has the maximum value $(15+\sqrt{241})/12 \approx 2.5437$ at $p = 0$ and the minimum value $(31+\sqrt{881})/24 \approx 2.5284$ at $p = 1/2$. That is say, for different p ($0 \le p \le 1/2$), the limit of $\log E[i(PH_{n,p})]/6n$ has little difference.

3. Merrifield-Simmons Index of a Random Hexagon Chain

Similar to the phenylene chain PH_n, the hexagon chain HS_n can be obtained by adjoining to HS_{n-1} a hexagon. For this construction the following relations are easily obtained by Lemmas 1 and 2.

Lemma 6. *Let HS_n be denoted as a hexagon squeeze of a phenylene chain PH_n as in Figure 2; then for $n \ge 2$ one has*

$$\begin{aligned} i(HS_n) &= 3i(HS_{n-1}) \\ &\quad + 2\left[i\left(HS_{n-1}-a_{n-1}\right) + i\left(HS_{n-1}-b_{n-1}\right)\right] \\ &\quad + i\left(HS_{n-1}-a_{n-1}-b_{n-1}\right), \end{aligned}$$

$$i(HS_n - a) = \begin{cases} 3i(HS_{n-1}) + 2i(HS_{n-1} - b_{n-1}), & if\ a = t_n, \\ 2i(HS_{n-1}) + 2i(HS_{n-1} - a_{n-1}) & \\ \quad +i(HS_{n-1} - b_{n-1}) & \\ \quad +i(HS_{n-1} - a_{n-1} - b_{n-1}), & if\ a = u_n, \\ 2i(HS_{n-1}) + i(HS_{n-1} - a_{n-1}) & \\ \quad +2i(HS_{n-1} - b_{n-1}) & \\ \quad +i(HS_{n-1} - a_{n-1} - b_{n-1}), & if\ a = v_n, \\ 3i(HS_{n-1}) + 2i(HS_{n-1} - a_{n-1}), & if\ a = w_n, \end{cases}$$

$$i(HS_n - a - b) = \begin{cases} 2i(HS_{n-1}) + i(HS_{n-1} - b_{n-1}), & if\ a = t_n,\ b = u_n, \\ i(HS_{n-1}) + i(HS_{n-1} - a_{n-1}) & \\ \quad +i(HS_{n-1} - b_{n-1}) & \\ \quad +i(HS_{n-1} - a_{n-1} - b_{n-1}), & if\ a = u_n,\ b = v_n, \\ 2i(HS_{n-1}) + i(HS_{n-1} - a_{n-1}), & if\ a = v_n,\ b = w_n. \end{cases} \tag{15}$$

Proof. Consider

$$\begin{aligned} i(\mathrm{HS}_n) &= i(\mathrm{HS}_n - t_n) + i(\mathrm{HS}_n - t_n - a_{n-1} - u_n) \\ &= i(\mathrm{HS}_{n-1} \cup P_2) + i((\mathrm{HS}_{n-1} - b_{n-1}) \cup P_1) \\ &\quad + i((\mathrm{HS}_{n-1} - a_{n-1}) \cup P_1) \\ &\quad + i(\mathrm{HS}_{n-1} - a_{n-1} - b_{n-1}) \\ &= i(P_2)\, i(\mathrm{HS}_{n-1}) \\ &\quad + i(P_1)\,[i(\mathrm{HS}_{n-1} - b_{n-1}) + i(\mathrm{HS}_{n-1} - a_{n-1})] \\ &\quad + i(\mathrm{HS}_{n-1} - a_{n-1} - b_{n-1}) \\ &= 3i(\mathrm{HS}_{n-1}) \\ &\quad + 2\,[i(\mathrm{HS}_{n-1} - a_{n-1}) + i(\mathrm{HS}_{n-1} - b_{n-1})] \\ &\quad + i(\mathrm{HS}_{n-1} - a_{n-1} - b_{n-1}), \\ i(\mathrm{HS}_n - t_n) &= i(\mathrm{HS}_{n-1} \cup P_2) + i((\mathrm{HS}_{n-1} - b_{n-1}) \cup P_1) \\ &= i(P_2)\, i(\mathrm{HS}_{n-1}) + i(P_1)\, i(\mathrm{HS}_{n-1} - b_{n-1}) \\ &= 3i(\mathrm{HS}_{n-1}) + 2i(\mathrm{HS}_{n-1} - b_{n-1}), \\ i(\mathrm{HS}_n - u_n) &= i(\mathrm{HS}_n - u_n - t_n) \\ &\quad + i(\mathrm{HS}_{n-1} - u_n - t_n - a_{n-1}) \\ &= i(\mathrm{HS}_{n-1} \cup P_1) + i(\mathrm{HS}_{n-1} - b_{n-1}) \\ &\quad + i((\mathrm{HS}_{n-1} - a_{n-1}) \cup P_1) \\ &\quad + i(\mathrm{HS}_{n-1} - a_{n-1} - b_{n-1}) \\ &= i(P_1)\, i(\mathrm{HS}_{n-1}) + i(\mathrm{HS}_{n-1} - b_{n-1}) \\ &\quad + i(P_1)\, i(\mathrm{HS}_{n-1} - a_{n-1}) \\ &\quad + i(\mathrm{HS}_{n-1} - a_{n-1} - b_{n-1}) \\ &= 2i(\mathrm{HS}_{n-1}) + 2i(\mathrm{HS}_n - a_{n-1}) \\ &\quad + i(\mathrm{HS}_{n-1} - b_{n-1}) \\ &\quad + i(\mathrm{HS}_{n-1} - a_{n-1} - b_{n-1}), \\ i(\mathrm{HS}_n - t_n - u_n) &= i(\mathrm{HS}_{n-1} \cup P_1) + i(\mathrm{HS}_{n-1} - b_{n-1}) \\ &= i(P_1)\, i(\mathrm{HS}_{n-1}) + i(\mathrm{HS}_{n-1} - b_{n-1}) \\ &= 2i(\mathrm{HS}_{n-1}) + i(\mathrm{HS}_{n-1} - b_{n-1}), \\ i(\mathrm{HS}_n - u_n - v_n) &= i(\mathrm{HS}_n - u_n - v_n - t_n) \\ &\quad + i(\mathrm{HS}_n - u_n - v_n - t_n - a_{n-1}) \\ &= i(\mathrm{HS}_{n-1}) + i(\mathrm{HS}_{n-1} - b_{n-1}) \\ &\quad + i(\mathrm{HS}_{n-1} - a_{n-1}) \\ &\quad + i(\mathrm{HS}_{n-1} - a_{n-1} - b_{n-1}). \end{aligned} \tag{16}$$

By the symmetry,

$$\begin{aligned} i(\mathrm{HS}_n - v_n) &= 2i(\mathrm{HS}_{n-1}) + i(\mathrm{HS}_n - a_{n-1}) \\ &\quad + 2i(\mathrm{HS}_{n-1} - b_{n-1}) + i(\mathrm{HS}_{n-1} - a_{n-1} - b_{n-1}), \\ i(\mathrm{HS}_n - w_n) &= 3i(\mathrm{HS}_{n-1}) + 2i(\mathrm{HS}_{n-1} - a_{n-1}), \\ i(\mathrm{HS}_n - v_n - w_n) &= 2i(\mathrm{HS}_{n-1}) + i(\mathrm{HS}_{n-1} - a_{n-1}). \end{aligned} \tag{17}$$

For a random hexagon chain $\mathrm{HS}_{n,p}$, the Merrifield-Simmons indices $i(\mathrm{HS}_{n,p})$, $i(\mathrm{HS}_{n,p} - a_n)$, $i(\mathrm{HS}_{n,p} - b_n)$, and $i(\mathrm{HS}_{n,p} - a_n - b_n)$ are also random variables, and in not confusion circumstances we also denote their expected values by $I_n = E[i(\mathrm{HS}_{n,p})]$, $U_n = E[i(\mathrm{HS}_{n,p} - a_n)]$, $V_n = E[i(\mathrm{HS}_{n,p} - b_n)]$, and $W_n = E[i(\mathrm{HS}_{n,p} - a_n - b_n)]$, respectively. Then we immediately have that, for $n \geq 2$,

$$\begin{aligned} I_n &= 3I_{n-1} + 2\,[U_{n-1} + V_{n-1}] + W_{n-1}, \\ U_n &= pE\left[i\left(\mathrm{HS}_{n,p} - t_n\right)\right] + pE\left[i\left(\mathrm{HS}_{n,p} - v_n\right)\right] \\ &\quad + (1 - 2p)\, E\left[i\left(\mathrm{HS}_{n,p} - u_n\right)\right] \\ &= pE\left[3i\left(\mathrm{HS}_{n-1,p}\right) + 2i\left(\mathrm{HS}_{n-1,p} - b_{n-1}\right)\right] \end{aligned}$$

$$
\begin{aligned}
&+ pE\left[2i\left(\mathrm{HS}_{n-1,p}\right) + i\left(\mathrm{HS}_{n-1,p} - a_{n-1}\right)\right.\\
&\qquad + 2i\left(\mathrm{HS}_{n-1,p} - b_{n-1}\right)\\
&\qquad \left. + i\left(\mathrm{HS}_{n-1,p} - a_{n-1} - b_{n-1}\right)\right]\\
&+ (1-2p)\\
&\cdot E\left[2i\left(\mathrm{HS}_{n-1,p}\right)\right.\\
&\qquad + 2i\left(\mathrm{HS}_{n-1,p} - a_{n-1}\right) + i\left(\mathrm{HS}_{n-1,p} - b_{n-1}\right)\\
&\qquad \left. + i\left(\mathrm{HS}_{n-1,p} - a_{n-1} - b_{n-1}\right)\right]\\
&= (2+p)\, E\left[i\left(\mathrm{HS}_{n-1,p}\right)\right]\\
&\quad + (2-3p)\, E\left[i\left(\mathrm{HS}_{n-1,p} - a_{n-1}\right)\right]\\
&\quad + (1+2p)\, E\left[i\left(\mathrm{HS}_{n-1,p} - b_{n-1}\right)\right]\\
&\quad + (1-p)\, E\left[i\left(\mathrm{HS}_{n-1,p} - a_{n-1} - b_{n-1}\right)\right]\\
&= (2+p)\, I_{n-1} + (2-3p)\, U_{n-1}\\
&\quad + (1+2p)\, V_{n-1} + (1-p)\, W_{n-1},\\
W_n &= pE\left[i\left(\mathrm{HS}_{n,p} - t_n - u_n\right)\right] + pE\left[i\left(\mathrm{HS}_{n,p} - v_n - w_n\right)\right]\\
&\quad + (1-2p)\, E\left[i\left(\mathrm{HS}_{n,p} - u_n - v_n\right)\right]\\
&= pE\left[2i\left(\mathrm{HS}_{n-1,p}\right) + i\left(\mathrm{HS}_{n-1,p} - b_{n-1}\right)\right]\\
&\quad + p\left[2i\left(\mathrm{HS}_{n-1,p}\right) + i\left(\mathrm{HS}_{n-1,p} - a_{n-1}\right)\right]\\
&\quad + (1-2p)\, E\left[i\left(\mathrm{HS}_{n-1,p}\right) + i\left(\mathrm{HS}_{n-1,p} - b_{n-1}\right)\right.\\
&\qquad\qquad \left. + i\left(\mathrm{HS}_{n-1,p} - a_{n-1}\right)\right.\\
&\qquad\qquad \left. + i\left(\mathrm{HS}_{n-1,p} - a_{n-1} - b_{n-1}\right)\right]\\
&= (1+2p)\, E\left[i\left(\mathrm{HS}_{n-1,p}\right)\right]\\
&\quad + (1-p)\, E\left[i\left(\mathrm{HS}_{n-1,p} - a_{n-1}\right)\right]\\
&\quad + (1-p)\, E\left[i\left(\mathrm{HS}_{n-1,p} - b_{n-1}\right)\right]\\
&\quad + (1-2p)\, E\left[i\left(\mathrm{HS}_{n-1,p} - a_{n-1} - b_{n-1}\right)\right]\\
&= (1+2p)\, I_{n-1} + (1-p)\, U_{n-1}\\
&\quad + (1-p)\, V_{n-1} + (1-2p)\, W_{n-1}.
\end{aligned}
\tag{18}
$$

By the symmetry,

$$
\begin{aligned}
V_n = {} & (2+p)\, I_{n-1} + (1+2p)\, U_{n-1}\\
& + (2-3p)\, V_{n-1} + (1-p)\, W_{n-1}.
\end{aligned}
\tag{19}
$$

Just as above, we set

$$
\begin{aligned}
I(t) &= \sum_{n\geq 1} I_n t^n, \qquad U(t) = \sum_{n\geq 1} U_n t^n,\\
V(t) &= \sum_{n\geq 1} V_n t^n, \qquad W(t) = \sum_{n\geq 1} W_n t^n.
\end{aligned}
\tag{20}
$$

Then we have that

$$
\begin{aligned}
I(t) - 18t &= 3tI(t) + 2t\left[U(t) + V(t)\right] + tW(t),\\
U(t) - 13t &= (2+p)\, tI(t) + (2-3p)\, tU(t)\\
&\quad + (1+2p)\, tV(t) + (1-p)\, tW(t),\\
V(t) - 13t &= (2+p)\, tI(t) + (1+2p)\, tU(t)\\
&\quad + (2-3p)\, tV(t) + (1-p)\, tW(t),\\
W(t) - 8t &= (1+2p)\, tI(t) + (1-p)\, tU(t)\\
&\quad + (1-p)\, tV(t) + (1-2p)\, tW(t).
\end{aligned}
\tag{21}
$$

Recall that $I_1 = 18$, $U_1 = V_1 = 13$, and $W_1 = 8$.

Solving the equations, we have that

$$
\begin{aligned}
I(t) &= \frac{6t\left(3 - 2t + 9pt\right)}{1 - 7t + 6pt + 4t^2 - 36pt^2}\\
&= \frac{At}{1 - \left(\left(7 - 3p + \sqrt{33 + 30p + 9p^2}\right)/2\right)t}\\
&\quad + \frac{Bt}{1 - \left(\left(7 - 3p - \sqrt{33 + 30p + 9p^2}\right)/2\right)t},
\end{aligned}
\tag{22}
$$

where

$$
\begin{aligned}
A &= 9 + \frac{(59 - 9p)\sqrt{33 + 30p + 9p^2}}{33 + 30p + 9p^2},\\
B &= 9 - \frac{(59 - 9p)\sqrt{33 + 30p + 9p^2}}{33 + 30p + 9p^2}.
\end{aligned}
\tag{23}
$$

□

So we have the following result.

Theorem 7. *If $0 \leq p \leq 1/2$, then for $n \geq 2$ one has that*

$$
\begin{aligned}
E\left[i\left(HS_{n,p}\right)\right] &= A\left(\frac{7 - 3p + \sqrt{33 + 30p + 9p^2}}{2}\right)^{n-1}\\
&\quad + B\left(\frac{7 - 3p - \sqrt{33 + 30p + 9p^2}}{2}\right)^{n-1},
\end{aligned}
\tag{24}
$$

where

$$A = 9 + \frac{(59 - 9p)\sqrt{33 + 30p + 9p^2}}{33 + 30p + 9p^2},$$
$$B = 9 - \frac{(59 - 9p)\sqrt{33 + 30p + 9p^2}}{33 + 30p + 9p^2}. \tag{25}$$

Specifically, we have that

$$\begin{aligned} E\left[i\left(HS_{n,1/2}\right)\right] &= \left(9 + \frac{109\sqrt{201}}{201}\right)\left(\frac{11 + \sqrt{201}}{4}\right)^{n-1} \\ &\quad + \left(9 - \frac{109\sqrt{201}}{201}\right)\left(\frac{11 - \sqrt{201}}{4}\right)^{n-1}, \\ E\left[i\left(HS_{n,1/3}\right)\right] &= \left(9 + \frac{28\sqrt{11}}{11}\right)\left(3 + \sqrt{11}\right)^{n-1} \\ &\quad + \left(9 - \frac{28\sqrt{11}}{11}\right)\left(3 - \sqrt{11}\right)^{n-1}, \\ E\left[i\left(HS_{n,0}\right)\right] &= \left(9 + \frac{59\sqrt{33}}{33}\right)\left(\frac{7 + \sqrt{33}}{2}\right)^{n-1} \\ &\quad + \left(9 - \frac{59\sqrt{33}}{33}\right)\left(\frac{7 - \sqrt{33}}{2}\right)^{n-1}. \end{aligned} \tag{26}$$

The following corollary is easily obtained from Theorem 7 which gives the limit of $\log E[i(\mathrm{HS}_{n,p})]/|V(\mathrm{HS}_{n,p})|$ as $n \to +\infty$, where $V(\mathrm{HS}_{n,p})$ is the vertex set of $\mathrm{HS}_{n,p}$.

Corollary 8. *If $0 \le p \le 1/2$, then for $n \ge 2$, one has*

$$\begin{aligned} &\lim_{n \to +\infty} \frac{\log E\left[i\left(HS_{n,p}\right)\right]}{\left|V\left(HS_{n,p}\right)\right|} \\ &= \lim_{n \to +\infty} \frac{\log E\left[i\left(HS_{n,p}\right)\right]}{4n + 2} \\ &= \frac{7 - 3p + \sqrt{33 + 30p + 9p^2}}{8}. \end{aligned} \tag{27}$$

It is easy to check that $g(p) = (7-3p+\sqrt{33 + 30p + 9p^2})/8$ is a monotonic decreasing function on p, so the limit of $\log E[i(HS_{n,p})]/|V(HS_{n,p})|$ has the maximum value $(7 + \sqrt{33})/2 \approx 1.062$ at $p = 0$, and the minimum value $(11 + \sqrt{201})/4 \approx 1.049$ at $p = 1/2$. That is say, for different p $(0 \le p \le 1/2)$, the limit of $\log E[i(HS_{n,p})]/|V(HS_{n,p})|$ has little difference.

Conflict of Interests

The author declares that there is no conflict of interests regarding the publication of this paper.

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