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The Expected Values of Hosoya Index and Merrifield–Simmons Index of Random Hexagonal Cactus Chains

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Abstract

Hosoya index and Merrifield-Simmons index are two well-known topological descriptors that reflex some physical properties, such as boiling points and heat of formation, of benzenoid hydrocarbon compounds. In this paper, we establish the generating functions of the expected values of these two indices of random hexagonal cacti. This generalizes the results of Došlić and Måløy, published in Discrete Mathematics in 2010. By applying the ideas on meromorphic functions and the growth of power series coefficients, the asymptotic behaviors of these indices on the random cacti have been established.

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1 Introduction and motivation

Throughout this paper, we may let $G = (V, E)$ be a graph having the vertex set V and the edge set E. For a vertex $v \in V$, we say that v is a *cut vertex* of G if $G - v$ has more components than G. A maximal connected subgraph H of G such that H does not have a cut vertex is called a *block*. Hence, if G has a cut vertex, then H contains a cut vertex of G. A block B is an *end block* if B has exactly one cut vertex of G. A vertex subset $I \subseteq V$ is *independent* if any pair of vertices in I are not adjacent in G. An edge subset $M \subseteq E$ is *matching* if any two edges in M are not adjacent to a common vertex. A *cycle* of length k is denoted by C_k. A *regular hexagonal cactus chain* is a graph that has exactly two end blocks and all the blocks are C_6, hexagons. A regular hexagonal cactus G is said to be *ortho* if the two cut vertices of G that belong to the same non-end block are adjacent. A regular hexagonal cactus G is said to be *meta* if the two cut vertices of G that belong to the same non-end block are a pair of vertices at distance two. Further, a regular hexagonal cactus G is said to be *para* if the two cut vertices of G that belong to the same non-end block is a pair of vertices at distance three. For a non-negative integer n and non-negative real numbers a, b, c such that $a + b + c = 1$, a *random hexagonal cactus chain* $R_n(a, b, c)$ with n hexagons is defined as follows: when $n = 0$, $R_0(a, b, c)$ is the empty graph. When $n = 1$, $R_1(a, b, c)$ is a hexagon and, when $n = 2$, $R_2(a, b, c)$ is obtained from two hexagons by identifying one vertex of each. For $n \geq 3$, renaming hexagons if necessary, we label the names of hexagons of $R_{n-1}(a, b, c)$ by $1, ..., n-1$ consecutively along the cactus. Further, the graph $R_n(a, b, c)$ is obtained from $R_{n-1}(a, b, c)$ and a hexagon H by identifying a vertex of H with a vertex at distance one with the probability a or a vertex at distance two with the probability b or the vertex at distance three with the probability c from the cut vertex of the $(n-1)^{th}$ hexagon of $R_{n-1}(a, b, c)$.

Husimi [13] expanded Mayer and Mayer [14]'s book of Statistical Mechanics by generalizing cluster and irreducible integrals for the Theory of Condensation in 1952. Surprisingly, Uhlenbeck [24] found in the same year that Husimi's integrals can be represented by using graph structures.

These kinds of graphs were known as *Husimi trees* which are graphs whose each edge is in at most one cycle. In some study such as [8, 10, 22], it was found further that Husimi trees can be employed to clarify many of condensation phenomena. Husimi trees were first described in graph theory literature as *cacti* in 1973 when Harary and Palmer [9] printed their classical book on graph enumeration.

In 1971, Hosoya introduced, in his classical paper [11], a graph parameter called Z-index which is the total number of matchings of the graphs. Hosoya found that Z-index relates with boiling point of the graphs representing saturated hydrocarbons. Interestingly, Gutman et al. [6] found further that Z-index also relates with the important molecular graph descriptor called *graph energy*. This has attracted much attentions of graph theorists and has resulted in many studies to evaluate this index of graphs which has been well known in Hosoya index later. For some example of studies to find Hosoya index see [4, 7, 20, 25].

From the observation of Merrifield and Simmons in [15–18], physical properties of hydrocarbons are related to topological indices on graphs applied in chemistry which describe molecular structures such as the number of independent sets. Specifically, in [15], the number of independent sets of graphs representing alkanes varies inversely to the boiling points and heat of formations of the compounds. From then on, Merrifield-Simmons index is recognized as the number of independent sets of graphs representing molecular structures which have been researched by several graph theorists, see [2, 3, 19, 21] for example.

In 2010, Došlić and Måløy [3] established the generating functions of Hosoya index and Merrifield-Simmons index of ortho-, meta-, and para-hexagonal cactus chain. In the following, we let H_n be a hexagonal cactus chain of n hexagons, in particular, we let O_n, M_n and P_n be the ortho-, meta- and para-hexagonal cactus chain of n hexagons, respectively.

Theorem 1. *[3] For a non-negative integer n, let $O(x), M(x)$ and $P(x)$ be the generating functions of the number of matchings of O_n, M_n and P_n,* *respectively. Then*

$$O(x) = \frac{1+7x}{1-11x-26x^2}$$
$$M(x) = \frac{1+5x}{1-13x+10x^2}$$
$$P(x) = \frac{1+6x}{1-12x-8x^2}.$$

Theorem 2. *[3] For a non-negative integer n, let $\overline{O}(x), \overline{M}(x)$ and $\overline{P}(x)$ be the generating functions of the number of independent sets of O_n, M_n and P_n, respectively. Then*

$$\overline{O}(x) = \frac{2+2x}{1-8x-25x^2}$$
$$\overline{M}(x) = \frac{2-6x}{1-12x+11x^2}$$
$$\overline{P}(x) = \frac{2-2x}{1-10x-7x^2}.$$

In the same paper, the authors further established the structures of hexagonal cacti whose Hosoya and Merrifield-Simmons indices are minimum and maximum.

Theorem 3. *[3] For a hexagonal cactus chain H_n of n hexagons, we let $m(H_n)$ be the Hosoya index of H_n. Then*

$$m(M_n) \leq m(H_n) \leq m(O_n).$$

Theorem 4. *[3] For a hexagonal cactus chain H_n of n hexagons, we let $i(H_n)$ be the Merrifield-Simmons index of H_n. Then*

$$i(M_n) \leq i(H_n) \leq i(O_n).$$

For related works on finding Hosoya index and Merrrifield-Simmons index in random chain, Huang et al. [12] described exact formulas for the expected values of these indices of a random polyphenylene chain including n octagons. Chen et al. [1] established explicit expressions for the expected value of Merrifield-Simmons index of a random phenylene chain $PH_{n,p}$ and a random hexagonal chain $HS_{n,p}$ by using the method of the generating functions. The corresponding entropy constants are computed and the maximum and minimum values are obtained in both random systems. Very recently in 2022, Sun et al. [23] found the recurrence relations of the expected values of Hosoya index and Merrifield-Simmons index of a random cyclooctylene chains containing n octagons. By solving these recurrence relations, the formula of expected values of these indices were established.

In this paper, we establish generating functions of the expected values of Hosoya index and Merrifield-Simmons index of random hexagonal cactus chain. Some special cases of our results prove Theorems 1 and 2.

2 Main results

In this section, we present our theorems related to the expected values of Hosoya index and Merrifield-Simmons index of random hexagonal cactus chains. Our first theorem establishes generating function of expected values of Hosoya index of random hexagonal cactus chains.

Theorem 5. *For a non-negative integer n and non-negative real numbers a, b, c such that $a+b+c = 1$, we let $R_n(a, b, c)$ be a random hexagonal cactus chain with n hexagons. Further, we let $E(m_n(a, b, c))$ be the expected value of the number of matchings of $R_n(a, b, c)$ and $M_{a,b,c}(x)$ be the generating function of $E(m_n(a, b, c))$. Then*

$$\begin{aligned} M_{a,b,c}(x) &= \sum_{n=0}^{\infty} E(m_n(a,b,c))x^n \\ &= \frac{1 + 10x - 3ax - 5bx - 4cx}{1 - 8x - 3ax - 5bx - 4cx - 26ax^2 + 10bx^2 - 8cx^2}. \end{aligned}$$

By letting $a = 1, b = c = 0$ and $a = c = 0, b = 1$ and $a = b = 0, c = 1$, we have that the graph $R_n(a, b, c)$ becomes ortho-, meta- and para-hexagonal cactus chain, respectively. Thus, we have the following equations:

$$M_{1,0,0}(x) = O(x) = \frac{1+7x}{1-11x-26x^2}$$
$$M_{0,1,0}(x) = M(x) = \frac{1+5x}{1-13x+10x^2}$$
$$M_{0,0,1}(x) = P(x) = \frac{1+6x}{1-12x-8x^2}.$$

Hence, Theorem 5 generalizes Theorem 1.

Further, we determine the asymptotic behavior of $E(m_n(a,b,c))$. As the dominant singularity is at $-\frac{3a+5b+4c-\sigma_1+8}{52a-20b+16c}$ where σ_1 is given in the theorem below, we apply the subtraction of singularities by the principal part of the series expansion around the singularity [26] and obtain the result as follows:

Theorem 6. *If $E(m_n(a,b,c))$ is the expected value of the number of matchings of $R_n(a,b,c)$. Then,*
$E(m_n(a,b,c)) \approx$

$$\frac{\sigma_2 - 3a\sigma_1 - 5b\sigma_1 - 4c\sigma_1 + 9a^2 + 25b^2 + 16c^2 + 10\sigma_1 - 80}{(-\frac{3a+5b+4c-\sigma_1+8}{52a-20b+16c})^{n+1}(52a-20b+16c)\sigma_1}$$

where
$\sigma_1 = \sqrt{9a^2 + 30ab + 24ac + 152a + 25b^2 + 40bc + 40b + 16c^2 + 96c + 64}$
and $\sigma_2 = 46a - 30b + 8c + 30ab + 24ac + 40bc.$

It can be observed that the growth of the expected value follows the form $A^n\theta(n)$ [5] where the subexponential factor $\theta(n)$ is given by

$$\frac{\sigma_2 - 3a\sigma_1 - 5b\sigma_1 - 4c\sigma_1 + 9a^2 + 25b^2 + 16c^2 + 10\sigma_1 - 80}{-(3a+5b+4c-\sigma_1+8)\sigma_1}.$$

Then seeking extreme values for the growth function is implemented by fmincon in MATLAB with SQP algorithm considering a, b and c as non-negative variables constrained to $a+b+c=1$. As a result, the maximum of $m(R_n(a,b,c))$ can be reached at $a=1, b=0, c=0$ and the minimum of $m(R_n(a,b,c))$ at $a=0, b=1, c=0$. That is

$$m(M_n) \le m(H_n) \le m(O_n),$$

proving Theorem 3.

Theorem 7. *For a non-negative integer n and non-negative real numbers a, b, c such that $a + b + c = 1$, we let $R_n(a, b, c)$ be a random hexagonal cactus chain with n hexagons. Further, we let $E(i_n(a, b, c))$ be the expected value of the number of independent sets of $R_n(a, b, c)$ and $I_{a,b,c}(x)$ be the generating function of $E(i_n(a, b, c))$. Then*

$$\begin{aligned} I_{a,b,c}(x) &= \sum_{n=0}^{\infty} E(i_n(a, b, c))x^n \\ &= \frac{1 + 13x - 3ax - 7bx - 5cx + 25ax^2 - 11bx^2 + 7cx^2}{1 - 5x - 3ax - 7bx - 5cx - 25ax^2 + 11bx^2 - 7cx^2}. \end{aligned}$$

By letting $a = 1, b = c = 0$ and $a = c = 0, b = 1$ and $a = b = 0, c = 1$ the graph $R_n(a, b, c)$ becomes ortho-, meta- and para-hexagonal cactus chain, respectively. Thus, we have the following equations:

$$\begin{aligned} I_{1,0,0}(x) = \overline{O}(x) &= \frac{1 + 10x + 25x^2}{1 - 8x - 25x^2} \\ I_{0,1,0}(x) = \overline{M}(x) &= \frac{1 + 6x - 11x^2}{1 - 12x + 11x^2} \\ I_{0,0,1}(x) = \overline{P}(x) &= \frac{1 + 8x + 7x^2}{1 - 10x - 7x^2}. \end{aligned}$$

Hence, Theorem 7 completes Theorem 2.

Further, in a similar fasion to Theorem 6, we have the asymptotic behavior of $E(i_n(a, b, c))$ as follows:

Theorem 8. *If $E(i_n(a, b, c))$ is the expected value of the number of independent sets of $R_n(a, b, c)$. Then,*
$E(i_n(a, b, c)) \approx$

$$\frac{-3a\sigma_1 - 7b3a\sigma_1 - 5c3a\sigma_1 + 42ab + 30ac + 70bc + 4\sigma_1 + \sigma_3}{(-\frac{3a+7b+5c-\sigma_1+5}{2\sigma_2})^{n+1}\sigma_1\sigma_2}.$$

where

$\sigma_1 = \sqrt{9a^2 + 42ab + 30ac + 130a + 49b^2 + 70bc + 26b + 25c^2 + 78c + 25}$ *and* $\sigma_2 = 25a - 11b + 7c$ *and* $\sigma_3 = 9a^2 + 49b^2 + 25c^2 - 20 + 53a - 15b + 19c.$

Similarly, the obtained function with a, b, c as non-negative variables such that $a + b + c = 1$ has extreme values where the maximum of $i(R_n(a, b, c))$ can be reached at $a = 1, b = 0, c = 0$ and the minimum of $i(R_n(a, b, c))$ at $a = 0, b = 1, c = 0$. That is

$$i(M_n) \leq i(H_n) \leq i(O_n),$$

proving Theorem 4.

3 Proofs of main results

In this section, we prove Theorems 5 and 7. Firstly, we recall that, for non-negative real numbers a, b, c such that $a + b + c = 1$, the graph $R_0(a, b, c)$ is empty, the graph $R_1(a, b, c)$ is a hexagon and the graph $R_2(a, b, c)$ is obtained from two hexagons by identifying one vertex of each. For $n \geq 3$, the graph $R_n(a, b, c)$ is obtained from $R_{n-1}(a, b, c)$ and a hexagon H by identifying a vertex of H with a vertex at distance one with the probability a or a vertex at distance two with the probability b or the vertex at distance three with the probability c from the cut vertex of the $(n-1)^{th}$ hexagon of $R_{n-1}(a, b, c)$. Figure 1 shows examples of $R_n(a, b, c)$.

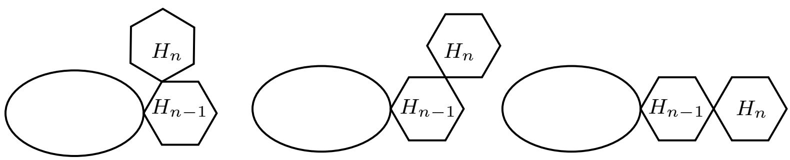

Figure 1. The graphs $R_n(a, b, c)$

In the figure, from left to right, a vertex of the hexagon H_n is identified with a vertex of the hexagon H_{n-1} with the probabilities a, b and c, respectively.

We further define three auxiliary graphs as follows. The graph $R'_n(a, b, c)$ is obtained from $R_n(a, b, c)$ and a path of length four $P_5 = x_1x_2x_3x_4x_5$

by identifying x_1 of P_5 to a vertex at distance one with the probability a, a vertex at distance two with the probability b and the vertex at distance three with the probability c from the cut vertex of the n^{th} hexagon of $R_n(a,b,c)$. Figure 2 illustrates examples of $R'_n(a,b,c)$. From left to right, x_1 of the path $x_1...x_5$ is identified with a vertex of the hexagon H_n with the probabilities a,b and c, respectively.

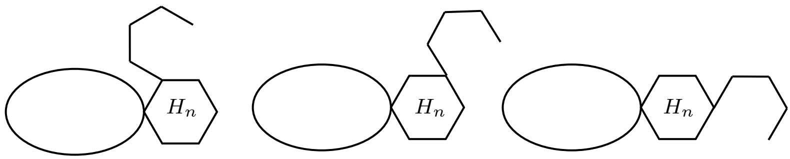

Figure 2. The graphs $R'_n(a,b,c)$

The graph $\tilde{R}_n(a,b,c)$ is obtained from $R_n(a,b,c)$ and a path of length four $P_5 = x_1x_2x_3x_4x_5$ by identifying x_2 of P_5 to a vertex at distance one with the probability a, a vertex at distance two with the probability b and the vertex at distance three with the probability c from the cut vertex of the n^{th} hexagon of $R_n(a,b,c)$. Figure 3 shows examples of $\tilde{R}_n(a,b,c)$. From left to right, x_2 of the path $x_1...x_5$ is identified with a vertex of the hexagon H_n with the probabilities a,b and c, respectively.

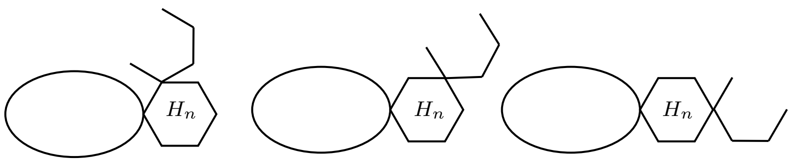

Figure 3. The graphs $\tilde{R}_n(a,b,c)$

The graph $\hat{R}_n(a,b,c)$ is obtained from $R_n(a,b,c)$ and a path of length four $P_5 = x_1x_2x_3x_4x_5$ by identifying x_3 of P_5 to a vertex at distance one with the probability a, a vertex at distance two with the probability b and the vertex at distance three with the probability c from the cut vertex of the n^{th} hexagon of $R_n(a,b,c)$. Figure 4 illustrates examples of $\hat{R}_n(a,b,c)$.

From left to right, x_3 of the path $x_1...x_5$ is identified with a vertex of the hexagon H_n with the probabilities a, b and c, respectively.

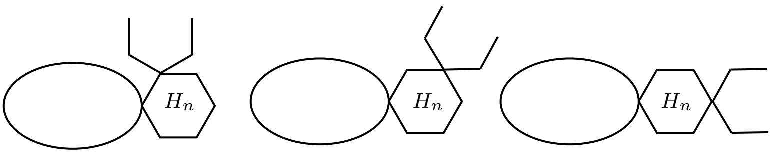

Figure 4. The graphs $\hat{R}_n(a, b, c)$

3.1 Hosoya index of random hexagonal cactus chains

In this subsection, we prove Theorem 5. Recall that

$E(m_n(a, b, c))$ is the expected value of the number of matchings of $R_n(a, b, c)$

$M_{a,b,c}(x)$ is the generating function of $E(m_n(a, b, c))$.

When there is no danger of confusion, we let $E(m_n)$ and $M(x)$ to denote $E(m_n(a, b, c))$ and $M_{a,b,c}(x)$, respectively. Thus,

$M(x) = \sum_{n=0}^{\infty} E(m_n)x^n$.

Similarly, we let $E(m'_n), E(\tilde{m}_n)$ and $E(\hat{m}_n)$ be the expected values of the number of matchings of $R'_n(a, b, c), \tilde{R}_n(a, b, c)$ and $\hat{R}_n(a, b, c)$, respectively. Further, we let $M'(x), \tilde{M}(x)$ and $\hat{M}(x)$ be the generating functions of $E(m'_n), E(\tilde{m}_n)$ and $E(\hat{m}_n)$, respectively. Therefore,

$M'(x) = \sum_{n=0}^{\infty} E(m'_n)x^n$

$\tilde{M}(x) = \sum_{n=0}^{\infty} E(\tilde{m}_n)x^n$

$\hat{M}(x) = \sum_{n=0}^{\infty} E(\hat{m}_n)x^n$.

Now, to prove Theorem 5, we will prove the following equations.

$$(1-8x)M(x) = 1 + 10x + 10ax^2M'(x) + 10bx^2\tilde{M}(x) + 10cx^2\hat{M}(x) \quad (1)$$

$$(1-3ax)M'(x) = 3 + 5M(x) + 3bx\tilde{M}(x) + 3cx\hat{M}(x) \quad (2)$$

$$(1-5bx)\tilde{M}(x) = 5 + 3M(x) + 5axM'(x) + 3cx\hat{M}(x) \quad (3)$$

$$(1-4cx)\hat{M}(x) = 4 + 4M(x) + 4axM'(x) + 4bx\tilde{M}(x) \quad (4)$$

Proof of Equation (1). We name the vertices of the n^{th} hexagon H_n of $R_n(a,b,c)$ by $h_1, h_2, ..., h_6$ clockwise with h_1 is the cut vertex containing in H_n (and in the $(n-1)^{th}$ hexagon H_{n-1}). Similarly, we name the vertices of H_{n-1} by $k_1, k_1, ..., k_6$ clockwise with k_1 is the cut vertex containing in H_{n-1}. Because $R_n(a,b,c)$ is a chain, $k_1 \neq h_1$. We distinguish three cases depending on the distance between h_1 and k_1 on H_{n-1}.

Case 1: h_1 is adjacent to k_1.

Thus, h_1 is either k_2 or k_6. Without loss of generality, we let $h_1 = k_2$. This case occurs with the probability a. We count the number of matchings due to the following subcases.

Subscase 1.1: The matchings that contain h_1h_2.

For any matching that contains h_1h_2, it cannot contain k_2k_3, k_1k_2, h_2h_3 and h_1h_6. Thus, the number of matchings in this subcase equals the number of matchings of the union of $R'_{n-2}(a,b,c)$ and the path $P_4 = h_3h_4h_5h_6$. Clearly, P_4 has 5 matchings. So, the expected value of the number of matchings in this subcase is $5E(m'_{n-2})$.

Subscase 1.2: The matchings that contain h_1h_6.

This subcase is symmetric to subcase 1.1. Thus, the expected value of the number of matchings in this subcase is $5E(m'_{n-2})$.

Subscase 1.3: The matchings that contain neither h_1h_2 nor h_1h_6.

The number of matchings in this subcase equals the number of matchings of the union of $R_{n-1}(a,b,c)$ and the path $P_5 = h_2h_3h_4h_5h_6$. Clearly, P_5 has 8 matchings. So, the expected value of the number of matchings in this subcase is $8E(m_{n-1})$.

From the three subcases, there are $10aE(m'_{n-2}) + 8aE(m_{n-1})$.

Case 2: h_1 is at distance two from k_1.

Thus, h_1 is either k_3 or k_5. Without loss of generality, we let $h_1 = k_3$. This case occurs with the probability b. We count the number of matchings due to the following subcases.

Subscase 2.1: The matchings that contain h_1h_2.

For any matching that contains h_1h_2, it cannot contain k_2k_3, k_3k_4, h_2h_3 and h_1h_6. Thus, the number of matchings in this subcase equals the number of matchings of the union of $\tilde{R}_{n-2}(a, b, c)$ and the path $P_4 = h_3h_4h_5h_6$. Clearly, P_4 has 5 matchings. So, the expected value of the number of matchings in this subcase is $5E(\tilde{m}_{n-2})$.

Subscase 2.2: The matchings that contain h_1h_6.

This subcase is symmetric to subcase 2.1. Thus, the expected value of the number of matchings in this subcase is $5E(\tilde{m}_{n-2})$.

Subscase 2.3: The matchings that contain neither h_1h_2 nor h_1h_6.

The number of matchings in this subcase equals the number of matchings of the union of $R_{n-1}(a, b, c)$ and the path $P_5 = h_2h_3h_4h_5h_6$. Clearly, P_5 has 8 matchings. So, the expected value of the number of matchings in this subcase is $8E(m_{n-1})$.

From the three subcases, there are $10bE(\tilde{m}_{n-2}) + 8bE(m_{n-1})$.

Case 3: h_1 is at distance three from k_1.

Thus, h_1 is k_4. This case occurs with the probability c. We count the number of matchings due to the following subcases.

Subscase 3.1: The matchings that contain h_1h_2.

For any matching that contains h_1h_2, it cannot contain k_4k_5, k_3k_4, h_2h_3 and h_1h_6. the number of matchings in this subcase equals the number of matchings of the union of $\hat{R}_{n-2}(a, b, c)$ and a path $P_4 = h_3h_4h_5h_6$. Clearly, P_4 has 5 matchings. So, the expected value of the number of matchings in this subcase is $5E(\hat{m}_{n-2})$.

Subscase 3.2: The matchings that contain h_1h_6.

This subcase is symmetric to subcase 3.1. Thus, the expected value of the number of matchings in this subcase is $5E(\hat{m}_{n-2})$.

Subscase 3.3: The matchings that contain neither h_1h_2 nor h_1h_6.

The number of matchings in this subcase equals the number of matchings of the union of $R_{n-1}(a,b,c)$ and the path $P_5 = h_2h_3h_4h_5h_6$. Clearly, P_5 has 8 matchings. So, the expected value of the number of matchings in this subcase is $8E(m_{n-1})$.

From the three subcases, there are $10cE(\hat{m}_{n-2}) + 8cE(m_{n-1})$. Therefore, from Cases $1, 2$ and 3, we have that

$$\begin{aligned}
E(m_n) &= 10aE(m'_{n-2}) + 8aE(m_{n-1}) + 10bE(\tilde{m}_{n-2}) + 8bE(m_{n-1}) \\
&\quad + 10cE(\hat{m}_{n-2}) + 8cE(m_{n-1}) \\
&= 8(a+b+c)E(m_{n-1}) + 10aE(m'_{n-2}) + 10bE(\tilde{m}_{n-2}) \\
&\quad + 10cE(\hat{m}_{n-2}) \\
&= 8E(m_{n-1}) + 10aE(m'_{n-2}) + 10bE(\tilde{m}_{n-2}) + 10cE(\hat{m}_{n-2}).
\end{aligned}$$

For $n \geq 2$, we multiply x^n throughout the above equation and sum over all n. We have that

$$\begin{aligned}
\sum_{n=2}^{\infty} E(m_n)x^n &= \sum_{n=2}^{\infty} 8E(m_{n-1})x^n + 10a\sum_{n=2}^{\infty} E(m'_{n-2})x^n \\
&\quad + 10b\sum_{n=2}^{\infty} E(\tilde{m}_{n-2})x^n + 10c\sum_{n=2}^{\infty} E(\hat{m}_{n-2})x^n
\end{aligned}$$

which implies that

$$\begin{aligned}
M(x) - E(m_0) - E(m_1)x &= 8x(M(x) - E(m_0)) + 10ax^2M'(x) \\
&\quad + 10bx^2\tilde{M}(x) + 10cx^2\hat{(M)}(x).
\end{aligned}$$

It can be checked that $E(m_0) = 1$ and $E(m_1) = 18$. Hence,

$$M(x) = 1 + 10x + 8xM(x) + 10ax^2M'(x) + 10bx^2\tilde{M}(x) + 10cx^2\hat{M}(x).$$

This proves Equation (1). ∎

Proof of Equation (2). Recall that $R'_n(a,b,c)$ is obtained from $R_n(a,b,c)$ and a path $P_5 = x_1x_2x_3x_4x_5$ by identifying x_1 with a vertex of the n^{th}

hexagon of $R_n(a,b,c)$. We name the vertices of the n^{th} hexagon H_n of $R'_n(a,b,c)$ by $h_1, h_2, ..., h_6$ clockwise with h_1 is the cut vertex containing in H_n (and in the $(n-1)^{th}$ hexagon H_{n-1}). By the definition of $R'_n(a,b,c)$, we have that $x_1 \neq h_1$. We distinguish three cases due to the distance between x_1 and h_1.

Case 1: x_1 is adjacent to h_1.

Thus, x_1 is either h_2 or h_6. Without loss of generality, we let $x_1 = h_2$. This case occurs with the probability a. We count the number of matchings due to the following subcases.

Subscase 1.1: The matchings that contain x_1x_2.

For any matching that contains x_1x_2, it cannot contain x_2x_3, h_1h_2 and h_2h_3. Thus, the number of matchings in this subcase equals the number of matchings of the union of $R'_{n-1}(a,b,c)$ and the path $x_3x_4x_5$. Clearly, $x_3x_4x_5$ has 3 matchings. So, the expected value of the number of matchings in this subcase is $3E(m'_{n-1})$.

Subscase 1.2: The matchings that do not contain x_1x_2.

The number of matchings in this subcase equals the number of matchings of the union of $R_n(a,b,c)$ and the path $x_2x_3x_4x_5$. Clearly, $x_2x_3x_4x_5$ has 5 matchings. So, the expected value of the number of matchings in this subcase is $5E(m_n)$.

From the two subcases, we have that there are $3aE(m'_{n-1}) + 5aE(m_n)$ from Case 1.

Case 2: x_1 is at distance two from h_1.

Thus, x_1 is either h_3 or h_5. Without loss of generality, we let $x_1 = h_3$. This case occurs with the probability b. We count the number of matchings due to the following subcases.

Subscase 2.1: The matchings that contain x_1x_2.

For any matching that contains x_1x_2, it cannot contain x_2x_3, h_3h_4 and h_2h_3. Thus, the number of matchings in this subcase equals the number of matchings of the union of $\tilde{R}_{n-1}(a,b,c)$ and the path $x_3x_4x_5$. Clearly, $x_3x_4x_5$ has 3 matchings. So, the expected value of the number of matchings in this subcase is $3E(\tilde{m}_{n-1})$.

Subscase 2.2: The matchings that do not contain x_1x_2.

The number of matchings in this subcase equals the number of matchings of the union of $R_n(a,b,c)$ and the path $x_2x_3x_4x_5$. Clearly, $x_2x_3x_4x_5$ has 5 matchings. So, the expected value of the number of matchings in this subcase is $5E(m_n)$.

From the two subcases, we have that there are $3bE(\tilde{m}_{n-1}) + 5bE(m_n)$ from Case 2.

Case 3: x_1 is at distance three from h_1.

Thus, x_1 is h_4. This case occurs with the probability c. We count the number of matchings due to the following subcases.

Subscase 3.1: The matchings that contain x_1x_2.

For any matching that contains x_1x_2, it cannot contain x_2x_3, h_3h_4 and h_4h_5. Thus, the number of matchings in this subcase equals the number of matchings of the union of $\hat{R}_{n-1}(a,b,c)$ and the path $x_3x_4x_5$. Clearly, $x_3x_4x_5$ has 3 matchings. So, the expected value of the number of matchings in this subcase is $3E(\hat{m}_{n-1})$.

Subscase 3.2: The matchings that do not contain x_1x_2.

The number of matchings in this subcase equals the number of matchings of the union of $R_n(a,b,c)$ and the path $x_2x_3x_4x_5$. Clearly, $x_2x_3x_4x_5$ has 5 matchings. So, the expected value of the number of matchings in this subcase is $5E(m_n)$.

From the two subcases, there are $3cE(\hat{m}_{n-1}) + 5cE(m_n)$ from Case 3. Therefore, from Cases $1, 2$ and 3, we have that

$$
\begin{aligned}
E(m'_n) &= 3aE(m'_{n-1}) + 5aE(m_n) + 3bE(\tilde{m}_{n-1}) + 5bE(m_n) \\
&\quad + 3cE(\hat{m}_{n-1}) + 5cE(m_n) \\
&= 5(a+b+c)E(m_n) + 3aE(m'_{n-1}) + 3bE(\tilde{m}_{n-1}) + 3cE(\hat{m}_{n-1}) \\
&= 5E(m_n) + 3aE(m'_{n-1}) + 3bE(\tilde{m}_{n-1}) + 3cE(\hat{m}_{n-1}).
\end{aligned}
$$

For $n \geq 1$, we multiply x^n throughout the above equation and sum over

all n. We have that

$$\sum_{n=1}^{\infty} E(m'_n)x^n = \sum_{n=1}^{\infty} 5E(m_n)x^n + 3a\sum_{n=1}^{\infty} E(m'_{n-1})x^n + 3b\sum_{n=1}^{\infty} E(\tilde{m}_{n-1})x^n + 3c\sum_{n=1}^{\infty} E(\hat{m}_{n-1})x^n$$

which implies that

$$M'(x) - E(m'_0) = 5(M(x) - E(m_0)) + 3axM'(x) + 3bx\tilde{M}(x) + 3cx\hat{M}(x).$$

Note that $E(m'_0)$ is the number of matchings of path of 5 vertices while $E(m_0)$ is the number of matching of size 0, the empty set, of the empty graph. Thus, $E(m'_0) = 8$ and $E(m_0) = 1$. Hence,

$$M'(x) = 3 + 5M(x) + 3axM'(x) + 3bx\tilde{M}(x) + 3cx\hat{M}(x).$$

This proves Equation (2). ■

Proof of Equation (3). Recall that $\tilde{R}_n(a,b,c)$ is obtained from $R_n(a,b,c)$ and a path $P_5 = x_1x_2x_3x_4x_5$ by identifying x_2 with a vertex of the n^{th} hexagon of $R_n(a,b,c)$. We name the vertices of the n^{th} hexagon H_n of $\tilde{R}_n(a,b,c)$ by $h_1, h_2, ..., h_6$ clockwise with h_1 is the cut vertex containing in H_n (and in the $(n-1)^{th}$ hexagon H_{n-1}). By the definition of $\tilde{R}_n(a,b,c)$, we have that $x_2 \neq h_1$. We distinguish three cases due to the distance between x_2 and h_1.

Case 1: x_2 is adjacent to h_1.

Thus, x_2 is either h_2 or h_6. Without loss of generality, we let $x_2 = h_2$. This case occurs with the probability a. We count the number of matchings due to the following subcases.

Subscase 1.1: The matchings that contain x_1x_2.

For any matching that contains x_1x_2, it cannot contain x_2x_3, h_1h_2 and h_2h_3. Thus, the number of matchings in this subcase equals the number of matchings of the union of $R'_{n-1}(a,b,c)$ and the path $P_3 = x_3x_4x_5$. Clearly, P_3 has 3 matchings. So, the expected value of the number of matchings in this subcase is $3E(m'_{n-1})$.

Subscase 1.2: The matchings that contain x_2x_3.

For any matching that contains x_2x_3, it cannot contain x_1x_2, x_3x_4, h_1h_2 and h_2h_3. Thus, the number of matchings in this subcase equals the number of matchings of the union of $R'_{n-1}(a,b,c)$, the vertex x_1 and the path $P_2 = x_4x_5$. Clearly, P_2 has 2 matchings. So, the expected value of the number of matchings in this subcase is $2E(m'_{n-1})$.

Subscase 1.3: The matchings that contain neither x_1x_2 nor x_2x_3.

The number of matchings in this subcase equals the number of matchings of the union of $R_n(a,b,c)$ and the path $P_3 = x_3x_4x_5$. Clearly, P_3 has 3 matchings. So, the expected value of the number of matchings in this subcase is $3E(m_n)$.

From the three subcases, we have that there are $5aE(m'_{n-1})+3aE(m_n)$.

Case 2: x_2 is at distance two from h_1.

Thus, x_2 is either h_3 or h_5. Without loss of generality, we let $x_2 = h_3$. This case occurs with the probability b. We count the number of matchings due to the following subcases.

Subscase 2.1: The matchings that contain x_1x_2.

For any matching that contains x_1x_2, it cannot contain x_2x_3, h_2h_3 and h_3h_4. Thus, the number of matchings in this subcase equals the number of matchings of the union of $\tilde{R}_{n-1}(a,b,c)$ and the path $P_3 = x_3x_4x_5$. Clearly, P_3 has 3 matchings. So, the expected value of the number of matchings in this subcase is $3E(\tilde{m}_{n-1})$.

Subscase 2.2: The matchings that contain x_2x_3.

For any matching that contains x_2x_3, it cannot contain x_1x_2, x_3x_4, h_3h_4 and h_2h_3. Thus, the number of matchings in this subcase equals the number of matchings of the union of $\tilde{R}_{n-1}(a,b,c)$, the vertex x_1 and the path $P_2 = x_4x_5$. Clearly, P_2 has 2 matchings. So, the expected value of the number of matchings in this subcase is $2E(\tilde{m}_{n-1})$.

Subscase 2.3: The matchings that contain neither x_1x_2 nor x_2x_3.

The number of matchings in this subcase equals the number of matchings of the union of $R_n(a,b,c)$ and the path $P_3 = x_3x_4x_5$. Clearly, P_3 has

3 matchings. So, the expected value of the number of matchings in this subcase is $3E(m_n)$.

From the three subcases, we have that there are $5bE(\tilde{m}_{n-1})+3bE(m_n)$.

Case 3: x_2 is at distance three from h_1.

Thus, x_2 is h_4. This case occurs with the probability c. We count the number of matchings due to the following subcases.

Subscase 3.1: The matchings that contain x_1x_2.

For any matching that contains x_1x_2, it cannot contain x_2x_3, h_3h_4 and h_4h_5. Thus, the number of matchings in this subcase equals the number of matchings of the union of $\hat{R}_{n-1}(a,b,c)$ and the path $P_3 = x_3x_4x_5$. Clearly, P_3 has 3 matchings. So, the expected value of the number of matchings in this subcase is $3E(\hat{m}_{n-1})$.

Subscase 3.2: The matchings that contain x_2x_3.

For any matching that contains x_2x_3, it cannot contain x_1x_2, x_3x_4, h_3h_4 and h_4h_5. Thus, the number of matchings in this subcase equals the number of matchings of the union of $\hat{R}_{n-1}(a,b,c)$, the vertex x_1 and the path $P_2 = x_4x_5$. Clearly, P_2 has 2 matchings. So, the expected value of the number of matchings in this subcase is $2E(\hat{m}_{n-1})$.

Subscase 3.3: The matchings that contain neither x_1x_2 nor x_2x_3.

The number of matchings in this subcase equals the number of matchings of the union of $R_n(a,b,c)$ and the path $P_3 = x_3x_4x_5$. Clearly, P_3 has 3 matchings. So, the expected value of the number of matchings in this subcase is $3E(m_n)$.

From the three subcases, we have that there are $5cE(\hat{m}_{n-1})+3cE(m_n)$. Therefore, from Cases 1, 2 and 3, we have that

$$\begin{aligned}
E(\tilde{m}_n) &= 5aE(m'_{n-1}) + 3aE(m_n) + 5bE(\tilde{m}_{n-1}) + 3bE(m_n) + 5cE(\hat{m}_{n-1}) \\
&\quad + 3cE(m_n)) \\
&= 3(a+b+c)E(m_n) + 5aE(m'_{n-1}) + 5bE(\tilde{m}_{n-1}) + 5cE(\hat{m}_{n-1}) \\
&= 3E(m_n) + 5aE(m'_{n-1}) + 5bE(\tilde{m}_{n-1}) + 5cE(\hat{m}_{n-1}).
\end{aligned}$$

For $n \geq 1$, we multiply x^n throughout the above equation and sum over

all n. We have that

$$\sum_{n=1}^{\infty} E(\tilde{m}_n)x^n = \sum_{n=1}^{\infty} 3E(m_n)x^n + 5a\sum_{n=1}^{\infty} E(m'_{n-1})x^n + 5b\sum_{n=1}^{\infty} E(\tilde{m}_{n-1})x^n + 5c\sum_{n=1}^{\infty} E(\hat{m}_{n-1})x^n$$

which implies that

$$\tilde{M}(x) - E(\tilde{m}_0) = 3(M(x) - E(m_0)) + 5axM'(x) + 5bx\tilde{M}(x) + 5cx\hat{M}(x).$$

Note that $E(\tilde{m}_0)$ is the number of matchings of path of 5 vertices while $E(m_0)$ is the number of matching of size 0, the empty set, of the empty graph. Thus, $E(\tilde{m}_0) = 8$ and $E(m_0) = 1$. Hence,

$$\tilde{M}(x) = 5 + 3M(x) + 5axM'(x) + 5bx\tilde{M}(x) + 5cx\hat{M}(x).$$

This proves Equation (3). ■

Proof of Equation (4). Recall that $\hat{R}_n(a, b, c)$ is obtained from $R_n(a, b, c)$ and a path $P_5 = x_1x_2x_3x_4x_5$ by identifying x_3 with a vertex of the n^{th} hexagon of $R_n(a, b, c)$. We name the vertices of the n^{th} hexagon H_n of $\hat{R}_n(a, b, c)$ by $h_1, h_2, ..., h_6$ clockwise with h_1 is the cut vertex containing in H_n (and in the $(n-1)^{th}$ hexagon H_{n-1}). By the definition of $\hat{R}_n(a, b, c)$, we have that $x_3 \neq h_1$. We distinguish three cases due to the distance between x_3 and h_1.

Case 1: x_3 is adjacent to h_1.

Thus, x_3 is either h_2 or h_6. Without loss of generality, we let $x_3 = h_2$. This case occurs with the probability a. We count the number of matchings due to the following subcases.

Subscase 1.1: The matchings that contain x_2x_3.

For any matching that contains x_2x_3, it cannot contain x_1x_2, x_3x_4, h_1h_2 and h_2h_3. Thus, the number of matchings in this subcase equals the number of matchings of the union of $R'_{n-1}(a, b, c)$, the vertex x_1 and the path $P_2 = x_4x_5$. Clearly, P_2 has 2 matchings. So, the expected value of the number of matchings in this subcase is $2E(m'_{n-1})$.

Subscase 1.2: The matchings that contain x_3x_4.

For any matching that contains x_3x_4, it cannot contain x_2x_3, x_4x_5, h_1h_2 and h_2h_3. Thus, the number of matchings in this subcase equals the number of matchings of the union of $R'_{n-1}(a,b,c)$, the vertex x_5 and the path x_1x_2. Clearly, x_1x_2 has 2 matchings. So, the expected value of the number of matchings in this subcase is $2E(m'_{n-1})$.

Subscase 1.3: The matchings that contain neither x_2x_3 nor x_3x_4.

The number of matchings in this subcase equals the number of matchings of the union of $R_n(a,b,c)$, the paths x_1x_2 and x_4x_5 . Clearly, x_1x_2 and x_4x_5 has 4 matchings. So, the expected value of the number of matchings in this subcase is $4E(m_n)$.

From the three subcases, we have that there are $4aE(m'_{n-1})+4aE(m_n)$.

Case 2: x_3 is at distance two from h_1.

Thus, x_3 is either h_3 or h_5. Without loss of generality, we let $x_3 = h_3$. This case occurs with the probability b. We count the number of matchings due to the following subcases.

Subscase 2.1: The matchings that contain x_2x_3.

For any matching that contains x_2x_3, it cannot contain x_1x_2, x_3x_4, h_2h_3 and h_3h_4. Thus, the number of matchings in this subcase equals the number of matchings of the union of $\tilde{R}_{n-1}(a,b,c)$, the vertex x_1 and the path x_4x_5. Clearly, x_4x_5 has 2 matchings. So, the expected value of the number of matchings in this subcase is $2E(\tilde{m}_{n-1})$.

Subscase 2.2: The matchings that contain x_3x_4.

For any matching that contains x_3x_4, it cannot contain x_2x_3, x_4x_5, h_2h_3 and h_3h_4. Thus, the number of matchings in this subcase equals the number of matchings of the union of $\tilde{R}_{n-1}(a,b,c)$, the vertex x_5 and the path x_1x_2. Clearly, x_1x_2 has 2 matchings. So, the expected value of the number of matchings in this subcase is $2E(\tilde{m}_{n-1})$.

Subscase 2.3: The matchings that contain neither x_2x_3 nor x_3x_4.

The number of matchings in this subcase equals the number of matchings of the union of $R_n(a,b,c)$, the paths x_1x_2 and x_4x_5 . Clearly, x_1x_2

and x_4x_5 has 4 matchings. So, the expected value of the number of matchings in this subcase is $4E(m_n)$.

From the three subcases, we have that there are $4bE(\tilde{m}_{n-1})+4bE(m_n)$.

Case 3: x_3 is at distance three from h_1.

Thus, x_3 is h_4. This case occurs with the probability c. We count the number of matchings due to the following subcases.

Subscase 3.1: The matchings that contain x_2x_3.

For any matching that contains x_2x_3, it cannot contain x_1x_2, x_3x_4, h_3h_4 and h_4h_5. Thus, the number of matchings in this subcase equals the number of matchings of the union of $\hat{R}_{n-1}(a,b,c)$, the vertex x_1 and the path x_4x_5. Clearly, x_4x_5 has 2 matchings. So, the expected value of the number of matchings in this subcase is $2E(\hat{m}_{n-1})$.

Subscase 3.2: The matchings that contain x_3x_4.

For any matching that contains x_3x_4, it cannot contain x_2x_3, x_4x_5, h_3h_4 and h_4h_5. Thus, the number of matchings in this subcase equals the number of matchings of the union of $\hat{R}_{n-1}(a,b,c)$, the vertex x_5 and the path x_1x_2. Clearly, x_1x_2 has 2 matchings. So, the expected value of the number of matchings in this subcase is $2E(\hat{m}_{n-1})$.

Subscase 3.3: The matchings that contain neither x_2x_3 nor x_3x_4.

The number of matchings in this subcase equals the number of matchings of the union of $R_n(a,b,c)$, the paths x_1x_2 and x_4x_5 . Clearly, x_1x_2 and x_4x_5 has 4 matchings. So, the expected value of the number of matchings in this subcase is $4E(m_n)$.

From the three subcases, we have that there are $4cE(\hat{m}_{n-1})+4cE(m_n)$. Therefore, from Cases $1, 2$ and 3, we have that

$$\begin{aligned} E(\hat{m}_n) &= 4aE(m'_{n-1}) + 4aE(m_n) + 4bE(\tilde{m}_{n-1}) + 4bE(m_n) + 4cE(\hat{m}_{n-1}) \\ &\quad + 4cE(m_n) \\ &= 4(a+b+c)E(m_n) + 4aE(m'_{n-1}) + 4bE(\tilde{m}_{n-1}) + 4cE(\hat{m}_{n-1}) \\ &= 4E(m_n) + 4aE(m'_{n-1}) + 4bE(\tilde{m}_{n-1}) + 4cE(\hat{m}_{n-1}). \end{aligned}$$

For $n \geq 1$, we multiply x^n throughout the above equation and sum over

all n. We have that

$$\sum_{n=1}^{\infty} E(\hat{m}_n)x^n = \sum_{n=1}^{\infty} 4E(m_n)x^n + 4a\sum_{n=1}^{\infty} E(m'_{n-1})x^n + 4b\sum_{n=1}^{\infty} E(\tilde{m}_{n-1})x^n + 4c\sum_{n=1}^{\infty} E(\hat{m}_{n-1})x^n$$

which implies that

$$\hat{M}(x) - E(\hat{m}_0) = 4(M(x) - E(m_0)) + 4axM'(x) + 4bx\tilde{M}(x) + 4cx\hat{M}(x).$$

Note that $E(\hat{m}_0)$ is the number of matchings of path of 5 vertices while $E(m_0)$ is the number of matching of size 0, the empty set, of the empty graph. Thus, $E(\hat{m}_0) = 8$ and $E(m_0) = 1$. Hence,

$$\hat{M}(x) = 4 + 4M(x) + 4axM'(x) + 4bx\tilde{M}(x) + 4cx\hat{M}(x).$$

This proves Equation (4). ■

By Equations (1), (2), (3) and (4), it can be solved that

$$M(x) = \frac{1 + 10x - 3ax - 5bx - 4cx}{1 - 8x - 3ax - 5bx - 4cx - 26ax^2 + 10bx^2 - 8cx^2}.$$

This proves Theorem 5. ■

3.2 Merrifield-Simmons index of random hexagonal cactus chains

In this subsection, we prove Theorem 7. Recall that

$E(i_n(a,b,c))$ is the expected value of the number of independent sets of $R_n(a,b,c)$.

$I_{a,b,c}(x)$ is the generating function of $E(i_n(a,b,c))$.

When there is no danger of confusion, we let $E(i_n)$ to denote $E(i_n(a,b,c))$ and let $I(x)$ to denote $I_{a,b,c}(x)$. Thus,

$I(x) = \sum_{n=0}^{\infty} E(i_n)x^n$.

Similarly, we let $E(i'_n), E(\tilde{i}_n)$ and $E(\hat{i}_n)$ be the expected values of the number of independent sets of $R'_n(a,b,c), \tilde{R}_n(a,b,c)$ and $\hat{R}_n(a,b,c)$, respectively. Further, we let $I'(x), \tilde{I}(x)$ and $\hat{I}(x)$ be the generating functions of $E(i'_n), E(\tilde{i}_n)$ and $E(\hat{i}_n)$, respectively. Therefore,

$I'(x) = \sum_{n=0}^{\infty} E(i'_n)x^n$

$\tilde{I}(x) = \sum_{n=0}^{\infty} E(\tilde{i}_n)x^n$

$\hat{I}(x) = \sum_{n=0}^{\infty} E(\hat{i}_n)x^n.$

Now, to prove Theorem 7, we need the following equations.

$$(1-5x)I(x) = 1 + 13x + 8ax^2 I'(x) + 8bx^2 \tilde{I}(x) + 8cx^2 \hat{I}(x) \tag{5}$$

$$(1-3ax)I'(x) = 8 + 5I(x) + 3bx\tilde{I}(x) + 3cx\hat{I}(x) \tag{6}$$

$$(1-7bx)\tilde{I}(x) = 10 + 3I(x) + 7axI'(x) + 7cx\hat{I}(x) \tag{7}$$

$$(1-5cx)\hat{I}(x) = 9 + 4I(x) + 5axI'(x) + 5bx\tilde{I}(x) \tag{8}$$

Because we can prove Equations (5) - (8) by similar arguments as Theorem 5, we omit the proofs of these equations.

By Equations (5), (6), (7) and (8), it can be solved that

$$I(x) = \frac{1 + 13x - 3ax - 7bx - 5cx + 25ax^2 - 11bx^2 + 7cx^2}{1 - 5x - 3ax - 7bx - 5cx - 25ax^2 + 11bx^2 - 7cx^2}.$$

This proves Theorem 7. ■

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