Iranian Journal of Mathematical chemistry

IJMC

DOI: 10.22052/IJMC.2025.257868.2080
Vol. 17, No. 2, 2026, pp. 179-199
Research Paper

Matching Polynomials and Independence Polynomials of Hexacyclic Systems

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Keywords:
Matching polynomial,
Independence polynomial,
Hexacyclic system.

AMS Subject Classification (2020):

05C09; 05C92; 05C30

Article History:
Received: 29 October 2025,
Accepted: 8 December 2025

Abstract

It is well established that matching and independence polynomials hold great significance in mathematical chemistry, serving as core tools to bridge the topological features of molecular graphs with quantifiable chemical properties. Against this backdrop, this paper focuses on computing the matching and independence polynomials of both hexacyclic systems and their Möbius counterparts. Building upon the research presented in "Matching polynomials and independence polynomials of benzenoid chains" [*MATCH Commun. Math. Comput. Chem.* **92** (2024) 779-809], we first develop methods to determine the matching and independence polynomials for an arbitrary hexacyclic system $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ and its Möbius counterpart $M_{\vartheta_1\vartheta_2\cdots\vartheta_h}$. Subsequently, computational formulas for the Hosoya index and Merrifield-Simmons index of both systems are derived.

1 Introduction

Polynomials associated with graphs have emerged as powerful tools for characterizing the structures and properties of (molecular) graphs. Among these, matching and independence polynomials occupy a prominent position, owing to their wide-ranging applications across diverse fields including theoretical chemistry, discrete mathematics, statistical physics, and computer science [1–3].

A matching in a graph is a set of edges in which no two edges share a common vertex. Let $m_k(G)$ denote the number of matchings of size k in G (where a matching of size 0 is the empty set, so $m_0(G) = 1$ for any graph G). For a graph G with n vertices, the matching polynomial [4, 5] is typically defined in two common (equivalent) forms:

$$\mu(G,x) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k m_k(G) x^{n-2k} \text{ and } \Psi(G,x) = \sum_{k=0}^{\lfloor n/2 \rfloor} m_k(G) x^k.$$

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Academic Editor: Tomislav Doslic

For convenience, in this paper, we adopt the version of the matching polynomial expressed in terms of the number of matchings without alternating signs, despite the signed version being more standard in algebraic graph theory, owing to its connections with eigenvalues of bipartite graphs and other polynomials. Clearly, the two versions can be converted into each other via the identity $\mu(G,x) = x^n\Psi(G, -1/x^2)$.

An independent set (or stable set) in a graph G is a set of vertices with no two vertices adjacent to each other, i.e., a subset of vertices where no two share an edge. Let $i_k(G)$ denote the number of independent sets of size k in G, where the empty set is counted as an independent set of size 0, so $i_0(G) = 1$ for any graph G. For a graph G, the independence polynomial [6] is defined as:

$$\Phi(G,x) = \sum_{k\geq 0} i_k(G)x^k.$$

The Hosoya index [7], also referred to as the z-index, holds particular value in investigating molecular structure-activity relationships and chemical similarity analysis [8]. For a graph G, the Hosoya index is defined as $z(G) = \sum_{k\geq 0} m_k(G)$. Notably, the Hosoya index of G can be derived from the matching polynomial $\Psi(G,x)$ by evaluating it at $x = 1$, i.e., $z(G) = \Psi(G,1)$. The Merrifield-Simmons index, alternatively called the σ-index, was introduced by R. E. Merrifield and H. E. Simmons [9]. For a graph G, this index is defined as $\sigma(G) = \sum_{k\geq 0} i_k(G)$, and similarly, it can be obtained from the independence polynomial $\Phi(G,x)$ by setting $x = 1$, i.e., $\sigma(G) = \Phi(G,1)$. Both the Hosoya index and Merrifield-Simmons index are important topological indices characterizing molecular graph structures. They primarily apply to QSAR and QSPR studies, linking molecular structures to diverse physicochemical properties and biological activities. Additionally, they aid drug design by supporting candidate compound screening and enhancing understanding of structure-property relationships.

A hexacyclic system with h hexagons can be formed by a sequence of hexagons $C_6^{(1)}$, $C_6^{(2)}$, $\ldots$, $C_6^{(h)}$ on a cylindrical strip, where each hexagon is connected to exactly two other hexagons via shared edges, and the vertices are shared by at most two hexagons. The total number of hexagons in a hexacyclic system is referred to as its length. For $i \in \{1,2,\ldots,h-1\}$, we denote the common edge shared by $C_6^{(i)}$ and $C_6^{(i+1)}$ as u_iv_i, and that shared by $C_6^{(h)}$ and $C_6^{(1)}$ as u_0v_0, where the vertices $u_0, u_1, u_2, \ldots, u_{h-1}$ lie on the same perimeter of the hexacyclic system, and $v_0, v_1, v_2, \ldots, v_{h-1}$ lie on the other perimeter. And the neighborhood of vertex u_0 in $C_6^{(h)}$ is $\{p, v_0\}$ while the neighborhood of vertex v_0 in $C_6^{(h)}$ is $\{q, u_0\}$. The distance $d(u,v)$ between two vertices u and v in a graph is defined as the length of the shortest path connecting u and v, where the length of a path is the number of edges in that path. For a hexacyclic system with h hexagons, with indices considered in the sense of modulo h (i.e., i is taken modulo h): if $d(u_{i-1},u_i) = d(v_{i-1},v_i) = 2$, then $C_6^{(i)}$ is called an α-type hexagon; if $d(u_{i-1},u_i) = d(v_{i-1},v_i) - 2 = 1$, then $C_6^{(i)}$ is called a β-type hexagon; if $d(u_{i-1},u_i) = d(v_{i-1},v_i) + 2 = 3$, then $C_6^{(i)}$ is called a γ-type hexagon. Thus, we may denote by $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ a hexacyclic system formed successively by ϑ_1-type, ϑ_2-type ,$\ldots$,ϑ_h-type hexagons, where $\vartheta_i \in \{\alpha,\beta,\gamma\}$ for $i \in \{1,2,\ldots,h\}$. Specifically, $F_{\alpha\alpha\cdots\alpha}$ is called a linear hexacyclic system, $F_{\beta\beta\cdots\beta}$ a helical hexacyclic system, and $F_{\beta\gamma\beta\gamma\cdots\beta\gamma}$ (for even h) or $F_{\beta\gamma\beta\gamma\cdots\beta\gamma\beta}$ (for odd h) a zig-zag hexacyclic system. Let $B_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ be the corresponding hexagonal chain created from hexacyclic system $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ by cutting the common edge u_0v_0, and the edge u_0v_0 is split into two edges within the hexagonal chain: uv, which belongs to $E(C_6^{(1)})$, and $u'v'$, which belongs to $E(C_6^{(h)})$. A hexacyclic system of length 12 and its corresponding hexagonal chain are depicted in Figure 1. For a hexacyclic system $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$, its Möbius counterpart $M_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ is derived from $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ by deleting edges pu_0 and qv_0 and adding edges pv_0 and qu_0. This $M_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ is also called a Möbius hexacyclic system, as it can be embedded in a Möbius strip. The Möbius counterpart of the hexacyclic system shown in Figure 1 is depicted in Figure 2.

Hexacyclic systems and Möbius hexacyclic systems are particularly relevant in chemical graph theory as they can be used to model a variety of molecular structures, including primitive coronoid systems, hollow hexagons, cylindrical (Hückel) and Möbius polyacenes. For linear hexacyclic systems and linear Möbius hexacyclic systems, the computation of some graph-spectrum-related parameters and substructure-related parameters has been well studied. However, relevant studies rarely extend to the cases of non-linear hexacyclic systems.

The transfer matrix technique has been proven highly effective in addressing counting problems related to substructure-based parameters in graphs. Notably, this method has recently enabled the successful resolution of counting and distribution problems concerning matchings and independent sets in certain chain-like molecular graphs–including benzenoid chains [10–12], phenylene chains [13], double hexagonal chains [14], primitive coronoid systems [15], among others. In this paper, we continue the work of [10] and investigate the computation of matchings

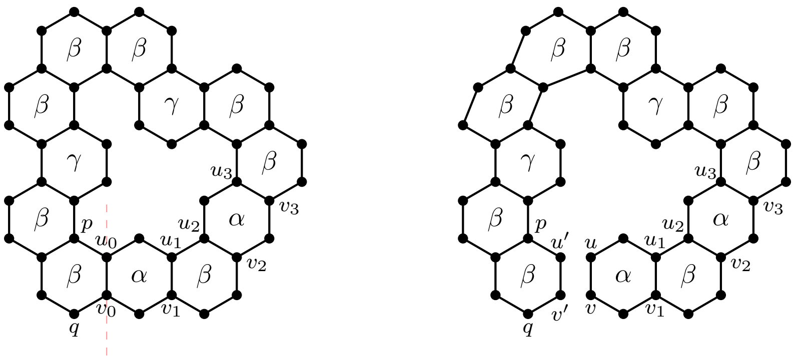

Figure 1: Hexacyclic system $F_{\alpha\beta\alpha\beta\beta\gamma\beta\beta\beta\gamma\beta\beta}$ and its corresponding hexagonal chain.

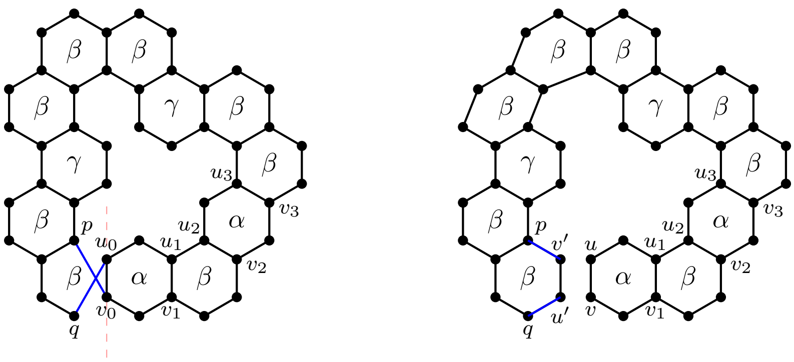

Figure 2: Möbius hexacyclic system $M_{\alpha\beta\alpha\beta\beta\gamma\beta\beta\beta\gamma\beta\beta}$ and its corresponding hexagonal chain.

and independent sets in hexacyclic systems and Möbius hexacyclic systems by using transfer matrix technique from the perspective of graph polynomials.

2 Preliminaries

All graphs addressed in this paper are simple and finite. For a graph G, its vertex set and edge set are denoted by $V(G)$ and $E(G)$, respectively. The neighborhood $N_G(v)$ of a vertex v in G consists of all vertices adjacent to v. The closed neighborhood of v, denoted by $N_G[v]$, includes v itself along with all its neighbors. When no ambiguity arises, the neighborhood and closed neighborhood of a vertex $v \in G$ are simplified to $N(v)$ and $N[v]$, respectively. For $v \in V(G)$, $G-v$ denotes the graph derived by removing vertex v and all its incident edges from G. Similarly, for $\{u, v\} \subseteq V(G)$, $G-u-v$ refers to the graph obtained by deleting both vertices u and v along with their incident edges. Moreover, if $uv \in E(G)$, then $G-uv$ represents the subgraph of G formed by removing the edge uv while retaining all vertices. We use $tr(\mathbf{M})$ to denote the trace of a square matrix $\mathbf{M}$. Let $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$ and $\mathbf{e}_4$ be the standard basis vectors in $\mathbb{R}^4$, i.e., $\mathbf{e}_1 = (1,0,0,0)^{\mathrm{T}}$, $\mathbf{e}_2 = (0,1,0,0)^{\mathrm{T}}$, $\mathbf{e}_3 = (0,0,1,0)^{\mathrm{T}}$, $\mathbf{e}_4 = (0,0,0,1)^{\mathrm{T}}$. We denote $\mathbf{E}_{(2,3)}$ as the elementary matrix obtained by interchanging the 2nd column and the 3rd column of the 4×4 identity matrix.

In what follows, we present some preliminary results related to matching and independence polynomials.

Lemma 2.1 ([5]). *(i) Let G be a graph with $uv \in E(G)$. Then $\Psi(G,x) = \Psi(G-uv,x) + x\Psi(G-u-v,x)$,*

(ii) Let G be a graph with t components $G_1, G_2, \ldots, G_t$. Then $\Psi(G,x) = \prod_{i=1}^{t} \Psi(G_i,x)$.

Lemma 2.2 ([6]). *(i) Let G be a graph with $u \in V(G)$. Then $\Phi(G,x) = \Phi(G-u,x) + x\Phi(G-N_G[u],x)$,*

(ii) Let G be a graph with t components $G_1, G_2, \ldots, G_t$. Then $\Phi(G,x) = \prod_{i=1}^{t} \Phi(G_i,x)$.

Definition 2.3 ([10]). Let G be a graph with $uv \in E(G)$. The vector $\Psi_{uv}(G,x)$ corresponding to the edge uv is given by

$$\Psi_{uv}(G,x) = (\Psi(G,x), \Psi(G-u,x), \Psi(G-v,x), \Psi(G-u-v,x))^{\mathrm{T}}.$$

The matrices $\mathbf{A}(x)$, $\mathbf{B}(x)$ and $\mathbf{C}(x)$ are defined as follows:

$$\mathbf{A}(x) = \begin{pmatrix} 1+3x+x^2 & x+2x^2 & x+2x^2 & x^2+x^3 \\ 1+x & x+x^2 & x & x^2 \\ 1+x & x & x+x^2 & x^2 \\ 1 & x & x & x^2 \end{pmatrix},$$

$$\mathbf{B}(x) = \begin{pmatrix} 1+3x+x^2 & x+2x^2 & x+2x^2 & x^2+x^3 \\ 1+2x & 0 & x+x^2 & 0 \\ 1+x & x+x^2 & x & x^2 \\ 1+x & 0 & x & 0 \end{pmatrix},$$

$$\mathbf{C}(x) = \begin{pmatrix} 1+3x+x^2 & x+2x^2 & x+2x^2 & x^2+x^3 \\ 1+x & x & x+x^2 & x^2 \\ 1+2x & x+x^2 & 0 & 0 \\ 1+x & x & 0 & 0 \end{pmatrix}.$$

Lemma 2.4 ([10]). *Let G be a graph obtained from the edge-coalescence of graph H and a hexagon, see Figure 3. Then* (i) *$\Psi_{uv}(G,x) = \mathbf{A}(x)\Psi_{st}(H,x)$;* (ii) *$\Psi_{uv}(G,x) = \mathbf{B}(x)\Psi_{ps}(H,x)$;* (iii) *$\Psi_{uv}(G,x) = \mathbf{C}(x)\Psi_{tq}(H,x)$.*

Definition 2.5 ([10])**.** Let G be a graph with $uv \in E(G)$. The vector $\Phi_{uv}(G,x)$ corresponding to the edge uv is given by

$$\Phi_{uv}(G,x) = (\Phi(G,x), \Phi(G-u,x), \Phi(G-v,x), \Phi(G-u-v,x))^{\mathrm{T}}.$$

The matrices $\mathbf{X}(x)$, $\mathbf{Y}(x)$ and $\mathbf{Z}(x)$ are defined as follows:

$$\mathbf{X}(x) = \begin{pmatrix} 1+2x & x+x^2 & x+x^2 & x^2 \\ 1+x & x+x^2 & x & x^2 \\ 1+x & x & x+x^2 & x^2 \\ 1 & x & x & x^2 \end{pmatrix},$$

$$\mathbf{Y}(x) = \begin{pmatrix} 1+2x & x+x^2 & x+x^2 & x^2 \\ 1+2x & 0 & x+x^2 & 0 \\ 1+x & x+x^2 & x & x^2 \\ 1+x & 0 & x & 0 \end{pmatrix},$$

$$\mathbf{Z}(x) = \begin{pmatrix} 1+2x & x+x^2 & x+x^2 & x^2 \\ 1+x & x & x+x^2 & x^2 \\ 1+2x & x+x^2 & 0 & 0 \\ 1+x & x & 0 & 0 \end{pmatrix}.$$

Lemma 2.6 ([10])**.** *Let G be a graph obtained from the edge-coalescence of graph H and a hexagon, see Figure 3. Then* (i) $\Phi_{uv}(G,x) = \mathbf{X}(x)\Phi_{st}(H,x)$*;* (ii) $\Phi_{uv}(G,x) = \mathbf{Y}(x)\Phi_{ps}(H,x)$*;* (iii) $\Phi_{uv}(G,x) = \mathbf{Z}(x)\Phi_{tq}(H,x)$*.*

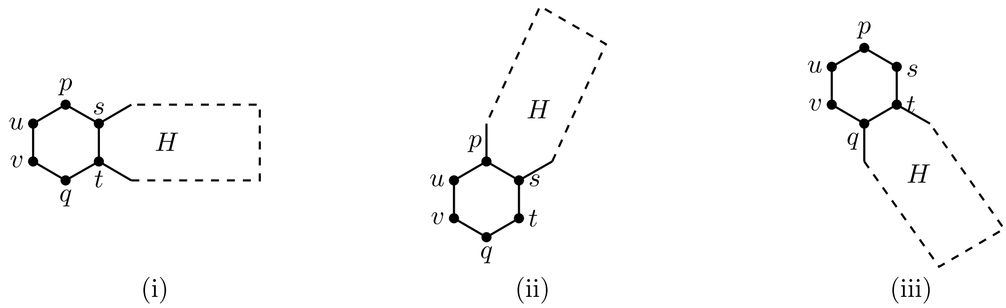

Figure 3: The graphs used in Lemma 2.4 and Lemma 2.6.

3 Main results

In this section, we present our main results, which are structured in two parts. Specifically, Subsection 3.1 is devoted to deriving the matching polynomials of any hexacyclic system $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ and its Möbius counterpart $M_{\vartheta_1\vartheta_2\cdots\vartheta_h}$, while Subsection 3.2 focuses on computing the independence polynomials of these two systems.

3.1 Matching polynomials of hexacyclic systems

In this subsection, we consider computing the matching polynomial for hexacyclic systems and their Möbius counterparts, and provide computational formulas for the Hosoya index of such systems.

Theorem 3.1. *For any hexacyclic system $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ with h hexagons, the matching polynomial of $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ is given by*

$$\Psi(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}, x) = tr\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big),$$

where $\mathbf{M}_i(x) = \mathbf{A}(x)$ if $\vartheta_i = \alpha$, $\mathbf{M}_i(x) = \mathbf{B}(x)$ if $\vartheta_i = \beta$, $\mathbf{M}_i(x) = \mathbf{C}(x)$ if $\vartheta_i = \gamma$, and $i \in \{1, 2, \ldots, h\}$.

Proof. Let $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ be a hexacyclic system composed of a sequence of hexagons $C_6^{(1)}$, $C_6^{(2)}$, ... , $C_6^{(h)}$. For $i \in \{1, 2, \ldots, h-1\}$, we denote the common edge of $C_6^{(i)}$ and $C_6^{(i+1)}$ as u_iv_i, and the common edge of $C_6^{(h)}$ and $C_6^{(1)}$ as u_0v_0. Moreover, the neighborhood of vertex u_0 in $C_6^{(h)}$ is $\{p, v_0\}$, while the neighborhood of vertex v_0 in $C_6^{(h)}$ is $\{q, u_0\}$. Let $B_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ be the corresponding hexagonal chain derived from the hexacyclic system $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ by cutting the common edge u_0v_0. This edge u_0v_0 is split into two edges uv and $u'v'$, both of which appear in its corresponding hexagonal chain, with $N(u') = \{p, v'\}$ and $N(v') = \{q, u'\}$. For $i \in \{1, 2, 3, \ldots, h\}$, we denote by $B_{\vartheta_i\vartheta_{i+1}\cdots\vartheta_h}$ the sub-chain of length $h - i + 1$ composed of the sequence of hexagons $C_6^{(i)}$, $C_6^{(i+1)}$, ... , $C_6^{(h)}$, and define the functional matrix $\mathbf{M}_i(x)$ as:

$$\mathbf{M}_i(x) = \begin{cases} \mathbf{A}(x), & \text{if } \vartheta_i = \alpha, \\ \mathbf{B}(x), & \text{if } \vartheta_i = \beta, \\ \mathbf{C}(x), & \text{if } \vartheta_i = \gamma. \end{cases}$$

By Definition 2.3 and Lemma 2.4, we can get that

$$\begin{aligned}\Psi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - u' - v', x) =& \mathbf{e}_1^{\mathrm{T}}\Psi_{uv}(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - u' - v', x) \\ =& \mathbf{e}_1^{\mathrm{T}}\mathbf{M}_1(x)\Psi_{u_1v_1}(B_{\vartheta_2\cdots\vartheta_h} - u' - v', x) \\ =& \mathbf{e}_1^{\mathrm{T}}\mathbf{M}_1(x)\mathbf{M}_2(x)\Psi_{u_2v_2}(B_{\vartheta_3\cdots\vartheta_h} - u' - v', x) \\ =& \cdots \\ =& \mathbf{e}_1^{\mathrm{T}}\Big(\prod_{i=1}^{h-1}\mathbf{M}_i(x)\Big)\Psi_{u_{h-1}v_{h-1}}(B_{\vartheta_h} - u' - v', x).\end{aligned}$$

Then, by Lemma 2.1, we can verify that the following equation holds.

$$\Psi_{u_{h-1}v_{h-1}}(B_{\vartheta_h} - u' - v', x) = \begin{cases} \mathbf{A}(x)\mathbf{e}_1, & \text{if } \vartheta_h = \alpha, \\ \mathbf{B}(x)\mathbf{e}_1, & \text{if } \vartheta_h = \beta, \\ \mathbf{C}(x)\mathbf{e}_1, & \text{if } \vartheta_h = \gamma. \end{cases}$$

Thus, we have

$$\Psi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - u' - v', x) = \mathbf{e}_1^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_1. \tag{1}$$

By Definition 2.3 and Lemma 2.4, we can get

$$\begin{aligned}\Psi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-p-u-u'-v',x) =&\mathbf{e}_2^{\mathrm{T}}\Psi_{uv}(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-p-u-u'-v',x)\\ =&\mathbf{e}_2^{\mathrm{T}}\mathbf{M}_1(x)\Psi_{u_1v_1}(B_{\vartheta_2\vartheta_3\cdots\vartheta_h}-p-u'-v',x)\\ =&\mathbf{e}_2^{\mathrm{T}}\mathbf{M}_1(x)\mathbf{M}_2(x)\Psi_{u_2v_2}(B_{\vartheta_3\cdots\vartheta_h}-p-u'-v',x)\\ =&\cdots\\ =&\mathbf{e}_2^{\mathrm{T}}\Big(\prod_{i=1}^{h-2}\mathbf{M}_i(x)\Big)\Psi_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h}-p-u'-v',x).\end{aligned}$$

If $\vartheta_{h-1}=\alpha$, then applying Lemma 2.1 we can verify that

$$x\Psi_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h}-p-u'-v',x)=\begin{cases}\mathbf{A}(x)\mathbf{A}(x)\mathbf{e}_2, & \text{if } \vartheta_h=\alpha,\\ \mathbf{A}(x)\mathbf{B}(x)\mathbf{e}_2, & \text{if } \vartheta_h=\beta,\\ \mathbf{A}(x)\mathbf{C}(x)\mathbf{e}_2, & \text{if } \vartheta_h=\gamma.\end{cases}$$

If $\vartheta_{h-1}=\beta$, then applying Lemma 2.1 we can verify that

$$x\Psi_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h}-p-u'-v',x)=\begin{cases}\mathbf{B}(x)\mathbf{A}(x)\mathbf{e}_2, & \text{if } \vartheta_h=\alpha,\\ \mathbf{B}(x)\mathbf{B}(x)\mathbf{e}_2, & \text{if } \vartheta_h=\beta,\\ \mathbf{B}(x)\mathbf{C}(x)\mathbf{e}_2, & \text{if } \vartheta_h=\gamma.\end{cases}$$

If $\vartheta_{h-1}=\gamma$, then applying Lemma 2.1 we can verify that

$$x\Psi_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h}-p-u'-v',x)=\begin{cases}\mathbf{C}(x)\mathbf{A}(x)\mathbf{e}_2, & \text{if } \vartheta_h=\alpha,\\ \mathbf{C}(x)\mathbf{B}(x)\mathbf{e}_2, & \text{if } \vartheta_h=\beta,\\ \mathbf{C}(x)\mathbf{C}(x)\mathbf{e}_2, & \text{if } \vartheta_h=\gamma.\end{cases}$$

Thus, we have

$$x\Psi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-p-u-u'-v',x)=\mathbf{e}_2^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_2. \tag{2}$$

Similarly, by Lemma 2.1 we can verify that

$$x\Psi_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h}-u'-q-v',x)=\mathbf{M}_{h-1}(x)\mathbf{M}_h(x)\mathbf{e}_3,$$

and

$$x^2\Psi_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h}-p-u'-q-v',x)=\mathbf{M}_{h-1}(x)\mathbf{M}_h(x)\mathbf{e}_4,$$

then we can further obtain

$$x\Psi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-u'-q-v-v',x)=\mathbf{e}_3^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_3, \tag{3}$$

and

$$x^2\Psi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-p-u-u'-q-v-v',x)=\mathbf{e}_4^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_4, \tag{4}$$

respectively. Therefore, applying Lemma 2.1 and in light of Equations (1)–(4), we have

$$\begin{aligned}\Psi(F_{\vartheta_1\vartheta_2\cdots\vartheta_h},x) =&\Psi(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}-pu_0,x)+x\Psi(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}-p-u_0,x)\\ =&\Psi(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}-pu_0-qv_0,x)+x\Psi(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}-pu_0-q-v_0,x)\\ &+x\Psi(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}-p-u_0-qv_0,x)\\ &+x^2\Psi(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}-p-u_0-q-v_0,x)\\ =&\Psi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-u'-v',x)+x\Psi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-p-u-u'-v',x)\\ &+x\Psi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-u'-q-v-v',x)\\ &+x^2\Psi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-p-u-u'-q-v-v',x)\\ =&\mathbf{e}_1^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_1+\mathbf{e}_2^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_2\\ &+\mathbf{e}_3^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_3+\mathbf{e}_4^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_4\\ =&tr\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big).\end{aligned}$$

The proof is complete. ■

As a concrete example, applying Theorem 3.1 allows one to readily get the matching polynomial of the hexacyclic system depicted in Figure 1.

Example 3.2. Let $G=F_{\alpha\beta\alpha\beta\beta\gamma\beta\beta\beta\gamma\beta\beta}$ be the hexacyclic system in Figure 1. Then

$$\begin{aligned}\Psi(G,x) =&tr\big(\mathbf{A}(x)\mathbf{B}(x)\mathbf{A}(x)\mathbf{B}(x)^2\mathbf{C}(x)\mathbf{B}(x)^3\mathbf{C}(x)\mathbf{B}(x)^2\big)\\ =&269x^{24}+26238x^{23}+836715x^{22}+12664967x^{21}+109254043x^{20}\\ &+598649980x^{19}+2235865832x^{18}+5975896530x^{17}+11836780846x^{16}\\ &+17828795484x^{15}+20816250079x^{14}+19110361487x^{13}+13938585640x^{12}\\ &+8134369990x^{11}+3813969108x^{10}+1438584394x^{9}+435776127x^{8}\\ &+105477643x^{7}+20212425x^{6}+3021407x^{5}+344323x^{4}\\ &+28854x^{3}+1674x^{2}+60x+1.\end{aligned}$$

Therefore, the number of matchings of all possible sizes on the hexacyclic system has been fully characterized.

The following conclusion provides a formula to calculate the Hosoya index for an arbitrary hexacyclic system.

Theorem 3.3. *For any hexacyclic system $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ with h hexagons, the Hosoya index of $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ is given by*

$$z(F_{\vartheta_1\vartheta_2\cdots\vartheta_h})=tr\Big(\prod_{i=1}^{h}\mathbf{M}_i\Big),$$

where $\mathbf{M}_i=\mathbf{A}$ if $\vartheta_i=\alpha$, $\mathbf{M}_i=\mathbf{B}$ if $\vartheta_i=\beta$, $\mathbf{M}_i=\mathbf{C}$ if $\vartheta_i=\gamma$, and

$$\mathbf{A}=\begin{pmatrix}5&3&3&2\\2&2&1&1\\2&1&2&1\\1&1&1&1\end{pmatrix},\ \mathbf{B}=\begin{pmatrix}5&3&3&2\\3&0&2&0\\2&2&1&1\\2&0&1&0\end{pmatrix},\ \mathbf{C}=\begin{pmatrix}5&3&3&2\\2&1&2&1\\3&2&0&0\\2&1&0&0\end{pmatrix}.$$

Proof. Given that for a graph G, $z(G) = \Psi(G, 1)$, the result can be straightforwardly derived from Theorem 3.1 when substituting $x = 1$. ■

Remark 1. Oz et al. [15] proposed a method to compute the Hosoya index of an arbitrary primitive coronoid system, which involves summing four products of 4×4 dimensional matrices with specific vectors.

Next, we proceed to investigate the computation of the matching polynomial for the Möbius hexacyclic systems.

Theorem 3.4. *Let $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ be a hexacyclic system with h hexagons. The matching polynomial of its Möbius counterpart $M_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ is given by*

$$\Psi(M_{\vartheta_1\vartheta_2\cdots\vartheta_h}, x) = tr\Big(\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{E}_{(2,3)}\Big),$$

where $\mathbf{E}_{(2,3)} = (\mathbf{e}_1, \mathbf{e}_3, \mathbf{e}_2, \mathbf{e}_4)$, $\mathbf{M}_i(x) = \mathbf{A}(x)$ if $\vartheta_i = \alpha$, $\mathbf{M}_i(x) = \mathbf{B}(x)$ if $\vartheta_i = \beta$, $\mathbf{M}_i(x) = \mathbf{C}(x)$ if $\vartheta_i = \gamma$.

Proof. Let $B_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ denote the corresponding hexagonal chain derived from the Möbius hexacyclic systems $M_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ by cutting along the common edge u_0v_0. This edge u_0v_0 is split into two edges uv and $u'v'$, both of which appear in this hexagonal chain, with $N(u') = \{q, v'\}$ and $N(v') = \{p, u'\}$. Similar to the proof of Theorem 3.1, by Lemma 2.1 we can get

$$\begin{aligned}
\Psi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - v' - u', x) &= \mathbf{e}_1^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_1,\\
x\Psi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - q - u - u' - v', x) &= \mathbf{e}_2^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_3,\\
x\Psi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - u' - p - v - v', x) &= \mathbf{e}_3^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_2,\\
x^2\Psi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - q - u - u' - p - v - v', x) &= \mathbf{e}_4^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_4,
\end{aligned}$$

where $\mathbf{M}_i(x) = \mathbf{A}(x)$ if $\vartheta_i = \alpha$, $\mathbf{M}_i(x) = \mathbf{B}(x)$ if $\vartheta_i = \beta$, $\mathbf{M}_i(x) = \mathbf{C}(x)$ if $\vartheta_i = \gamma$.

Then we have

$$\begin{aligned}
\Psi(M_{\vartheta_1\vartheta_2\cdots\vartheta_h},x) =&\Psi(M_{\vartheta_1\vartheta_2\cdots\vartheta_h}-qu_0,x)+x\Psi(M_{\vartheta_1\vartheta_2\cdots\vartheta_h}-u_0-q,x)\\
=&\Psi(M_{\vartheta_1\vartheta_2\cdots\vartheta_h}-qu_0-pv_0,x)+x\Psi(M_{\vartheta_1\vartheta_2\cdots\vartheta_h}-qu_0-p-v_0,x)\\
&+x\Psi(M_{\vartheta_1\vartheta_2\cdots\vartheta_h}-q-u_0-pv_0,x)\\
&+x^2\Psi(M_{\vartheta_1\vartheta_2\cdots\vartheta_h}-q-u_0-p-v_0,x)\\
=&\Psi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-v'-u',x)+x\Psi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-q-u-u'-v',x)\\
&+x\Psi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-u'-p-v-v',x)\\
&+x^2\Psi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-q-u-u'-p-v-v',x)\\
=&\mathbf{e}_1^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_1+\mathbf{e}_2^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_3\\
&+\mathbf{e}_3^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_2+\mathbf{e}_4^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_4\\
=&tr\bigg(\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{E}_{(2,3)}\bigg).
\end{aligned}$$

Therefore, we arrive at the desired result. ■

By Theorem 3.4, we can obtain the exact expression for the matching polynomial of the Möbius hexacyclic system depicted in Figure 2.

Example 3.5. For the Möbius hexacyclic system $G = M_{\alpha\beta\alpha\beta\beta\gamma\beta\beta\beta\gamma\beta\beta}$ as shown in Figure 2, applying Theorem 3.4 we can get

$$\begin{aligned}
\Psi(G,x) =& tr\big(\mathbf{A}(x)\mathbf{B}(x)\mathbf{A}(x)\mathbf{B}(x)^2\mathbf{C}(x)\mathbf{B}(x)^3\mathbf{C}(x)\mathbf{B}(x)^2\mathbf{E}_{2,3}\big)\\
=&267x^{24}+26221x^{23}+836759x^{22}+12670633x^{21}+109329908x^{20}\\
&+599110828x^{19}+2237455693x^{18}+5979363501x^{17}+11841870797x^{16}\\
&+17834030288x^{15}+20820117067x^{14}+19112442955x^{13}+13939406472x^{12}\\
&+8134606334x^{11}+3814018108x^{10}+1438591501x^{9}+435776810x^{8}\\
&+105477682x^{7}+20212426x^{6}+3021407x^{5}+344323x^{4}\\
&+28854x^{3}+1674x^{2}+60x+1.
\end{aligned}$$

Theorem 3.6. *For any hexacyclic system $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ with h hexagons, the Hosoya index of its Möbius counterpart $M_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ is given by*

$$z(M_{\vartheta_1\vartheta_2\cdots\vartheta_h}) = tr\bigg(\Big(\prod_{i=1}^{h}\mathbf{M}_i\Big)\mathbf{E}_{(2,3)}\bigg),$$

where $\mathbf{E}_{(2,3)} = (\mathbf{e}_1,\mathbf{e}_3,\mathbf{e}_2,\mathbf{e}_4)$, $\mathbf{M}_i = \mathbf{A}$ if $\vartheta_i = \alpha$, $\mathbf{M}_i = \mathbf{B}$ if $\vartheta_i = \beta$, $\mathbf{M}_i = \mathbf{C}$ if $\vartheta_i = \gamma$, and

$$\mathbf{A} = \begin{pmatrix}5&3&3&2\\2&2&1&1\\2&1&2&1\\1&1&1&1\end{pmatrix},\ \mathbf{B} = \begin{pmatrix}5&3&3&2\\3&0&2&0\\2&2&1&1\\2&0&1&0\end{pmatrix},\ \mathbf{C} = \begin{pmatrix}5&3&3&2\\2&1&2&1\\3&2&0&0\\2&1&0&0\end{pmatrix}.$$

Proof. The result can be straightforwardly derived from Theorem 3.4 by substituting $x = 1$. ■

The following three corollaries are immediate consequences of Theorems 3.3 and 3.6.

Corollary 3.7. *For a linear hexacyclic system $F_{\alpha\alpha\cdots\alpha}$ with $h \geq 3$ hexagons and its Möbius counterpart $M_{\alpha\alpha\cdots\alpha}$, we have $z(F_{\alpha\alpha\cdots\alpha}) = tr\big(\mathbf{A}^h\big)$ and $z(M_{\alpha\alpha\cdots\alpha}) = tr\big(\mathbf{A}^h\mathbf{E}_{(2,3)}\big)$.*

Corollary 3.8. *For a helical hexacyclic system $F_{\beta\beta\ldots\beta}$ with $h \geq 3$ hexagons and its Möbius counterpart $M_{\alpha\alpha\cdots\alpha}$, we have $z(F_{\beta\beta\ldots\beta}) = tr\big(\mathbf{B}^h\big)$ and $z(M_{\beta\beta\ldots\beta}) = tr\big(\mathbf{B}^h\mathbf{E}_{(2,3)}\big)$.*

Corollary 3.9. *For a zig-zag hexacyclic system $F_{\beta\gamma\beta\gamma\ldots}$ with $h \geq 3$ hexagonsits and its Möbius counterpart $M_{\beta\gamma\beta\gamma\ldots}$, we have*

- $z(F_{\beta\gamma\beta\gamma\ldots}) = \begin{cases} z(F_{\beta\gamma\beta\gamma\cdots\beta\gamma}) = tr\big((\mathbf{BC})^{\frac{h}{2}}\big), & \text{if } h \text{ is even,} \\ z(F_{\beta\gamma\beta\gamma\cdots\gamma\beta}) = tr\big((\mathbf{BC})^{\frac{h-1}{2}}\mathbf{B}\big), & \text{if } h \text{ is odd,} \end{cases}$
- $z(M_{\beta\gamma\beta\gamma\ldots}) = \begin{cases} z(M_{\beta\gamma\beta\gamma\cdots\beta\gamma}) = tr\big((\mathbf{BC})^{\frac{h}{2}}\mathbf{E}_{(2,3)}\big), & \text{if } h \text{ is even,} \\ z(M_{\beta\gamma\beta\gamma\cdots\gamma\beta}) = tr\big((\mathbf{BC})^{\frac{h-1}{2}}\mathbf{B}\mathbf{E}_{(2,3)}\big), & \text{if } h \text{ is odd.} \end{cases}$

3.2 Independence polynomials of hexacyclic systems

In this subsection, we focus on computing the independence polynomial for hexacyclic systems and their Möbius counterparts, and we present computational formulas for the Merrifield-Simmons index of these systems.

Theorem 3.10. *For any hexacyclic system $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ with h hexagons, the independence polynomial of $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ is given by*

$$\Phi(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}, x) = tr\bigg(\prod_{i=1}^{h}\mathbf{H}_i(x)\bigg),$$

where $\mathbf{H}_i(x) = \mathbf{X}(x)$ if $\vartheta_i = \alpha$, $\mathbf{H}_i(x) = \mathbf{Y}(x)$ if $\vartheta_i = \beta$, $\mathbf{H}_i(x) = \mathbf{Z}(x)$ if $\vartheta_i = \gamma$, and $i \in \{1, 2, \ldots, h\}$.

Proof. Let $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ be a hexacyclic system composed of a sequence of hexagons $C_6^{(1)}$, $C_6^{(2)}$, … , $C_6^{(h)}$, with $B_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ denoting its corresponding hexagonal chain derived from $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ by cutting along the common edge u_0v_0 shared by $C_6^{(h)}$ and $C_6^{(1)}$. This edge u_0v_0 is split into two edges uv and $u'v'$, both present in the latter, where $N(u') = \{p, v'\}$ and $N(v') = \{q, u'\}$. For $i \in \{1, 2, 3, \ldots, h\}$, we use $B_{\vartheta_i\vartheta_{i+1}\cdots\vartheta_h}$ to denote the sub-chain of length $h - i + 1$ formed by the sequence of hexagons $C_6^{(i)}$, $C_6^{(i+1)}$, … , $C_6^{(h)}$, and set the functional matrix $\mathbf{H}_i(x)$ as:

$$\mathbf{H}_i(x) = \begin{cases} \mathbf{X}(x), & \text{if } \vartheta_i = \alpha, \\ \mathbf{Y}(x), & \text{if } \vartheta_i = \beta, \\ \mathbf{Z}(x), & \text{if } \vartheta_i = \gamma. \end{cases}$$

By Definition 2.5 and Lemma 2.6, we can get that

$$\begin{aligned} \Phi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - p - q - u' - v', x) = {} & \mathbf{e}_1^{\mathrm{T}}\Phi_{uv}(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - p - q - u' - v', x) \\ = {} & \mathbf{e}_1^{\mathrm{T}}\mathbf{H}_1(x)\Psi_{u_1v_1}(B_{\vartheta_2\cdots\vartheta_h} - p - q - u' - v', x) \\ = {} & \mathbf{e}_1^{\mathrm{T}}\mathbf{H}_1(x)\mathbf{H}_2(x)\Psi_{u_2v_2}(B_{\vartheta_3\cdots\vartheta_h} - p - q - u' - v', x) \\ = {} & \cdots \\ = {} & \mathbf{e}_1^{\mathrm{T}}\bigg(\prod_{i=1}^{h-2}\mathbf{H}_i(x)\bigg)\Phi_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h} - p - q - u' - v', x). \end{aligned}$$

For the case of $\vartheta_{h-1} = \alpha$, applying Lemma 2.2, we can verify that

$$\Phi_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h} - p - q - u' - v', x) = \begin{cases} \mathbf{X}(x)\mathbf{X}(x)\mathbf{e}_1, & \text{if } \vartheta_h = \alpha, \\ \mathbf{X}(x)\mathbf{Y}(x)\mathbf{e}_1, & \text{if } \vartheta_h = \beta, \\ \mathbf{X}(x)\mathbf{Z}(x)\mathbf{e}_1, & \text{if } \vartheta_h = \gamma. \end{cases}$$

For the case of $\vartheta_{h-1} = \beta$, applying Lemma 2.2, we can verify that

$$\Phi_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h} - p - q - u' - v', x) = \begin{cases} \mathbf{Y}(x)\mathbf{X}(x)\mathbf{e}_1, & \text{if } \vartheta_h = \alpha, \\ \mathbf{Y}(x)\mathbf{Y}(x)\mathbf{e}_1, & \text{if } \vartheta_h = \beta, \\ \mathbf{Y}(x)\mathbf{Z}(x)\mathbf{e}_1, & \text{if } \vartheta_h = \gamma. \end{cases}$$

For the case of $\vartheta_{h-1} = \gamma$, applying Lemma 2.2, we can verify that

$$\Phi_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h} - p - q - u' - v', x) = \begin{cases} \mathbf{Z}(x)\mathbf{X}(x)\mathbf{e}_1, & \text{if } \vartheta_h = \alpha, \\ \mathbf{Z}(x)\mathbf{Y}(x)\mathbf{e}_1, & \text{if } \vartheta_h = \beta, \\ \mathbf{Z}(x)\mathbf{Z}(x)\mathbf{e}_1, & \text{if } \vartheta_h = \gamma. \end{cases}$$

Thus, we have

$$\Phi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - p - q - u' - v', x) = \mathbf{e}_1^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{H}_i(x)\Big)\mathbf{e}_1. \tag{5}$$

According to Lemma 2.2, we can obtain

$$x\Phi_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h} - N[p] - q - v', x) = \mathbf{H}_{h-1}(x)\mathbf{H}_h(x)\mathbf{e}_2,$$

$$x\Phi_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h} - p - N[q] - u', x) = \mathbf{H}_{h-1}(x)\mathbf{H}_h(x)\mathbf{e}_3,$$

and

$$x^2\Psi_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h} - N[p] - N[q], x) = \mathbf{H}_{h-1}(x)\mathbf{H}_h(x)\mathbf{e}_4,$$

then, by a similar analysis, we can further obtain

$$x\Phi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - N[p] - q - v' - u, x) = \mathbf{e}_2^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{H}_i(x)\Big)\mathbf{e}_2, \tag{6}$$

$$x\Phi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - p - N[q] - u' - v, x) = \mathbf{e}_3^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{H}_i(x)\Big)\mathbf{e}_3, \tag{7}$$

and

$$x^2\Phi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - N[p] - N[q] - u - v, x) = \mathbf{e}_4^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{H}_i(x)\Big)\mathbf{e}_4, \tag{8}$$

respectively.

Therefore, using Lemma 2.2 and Equations (5)–(8), we conclude that

$$\begin{aligned}\Phi(F_{\vartheta_1\vartheta_2\cdots\vartheta_h},x) =&\Phi(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}-p,x)+x\Phi(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}-N[p],x)\\ =&\Phi(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}-p-q,x)+x\Phi(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}-p-N[q],x)\\ &+x\Phi(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}-N[p]-q,x)+x^2\Phi(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}-N[p]-N[q],x)\\ =&\Phi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-p-q-u'-v',x)\\ &+x\Phi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-p-N[q]-u'-v,x)\\ &+x\Phi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-N[p]-q-v'-u,x)\\ &+x^2\Phi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-N[p]-N[q]-u-v,x)\\ =&\mathbf{e}_1^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{H}_i(x)\Big)\mathbf{e}_1+\mathbf{e}_2^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{H}_i(x)\Big)\mathbf{e}_2\\ &+\mathbf{e}_3^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{H}_i(x)\Big)\mathbf{e}_3+\mathbf{e}_4^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{H}_i(x)\Big)\mathbf{e}_4\\ =&tr\Big(\prod_{i=1}^{h}\mathbf{H}_i(x)\Big).\end{aligned}$$

This completes the proof. ■

As a concrete example, Theorem 3.6 can be readily applied to derive the independence polynomial of the hexacyclic system in Figure 1.

Example 3.11. Let $G=F_{\alpha\beta\alpha\beta\beta\gamma\beta\beta\beta\gamma\beta\beta}$ be the hexacyclic system in Figure 1. Then

$$\begin{aligned}\Phi(G,x)=&tr\big(\mathbf{X}(x)\mathbf{Y}(x)\mathbf{X}(x)\mathbf{Y}(x)^2\mathbf{Z}(x)\mathbf{Y}(x)^3\mathbf{Z}(x)\mathbf{Y}(x)^2\big)\\ =&2x^{24}+82x^{23}+2445x^{22}+43708x^{21}+490221x^{20}+3653028x^{19}\\ &+18852492x^{18}+69700196x^{17}+189887269x^{16}+390073090x^{15}\\ &+615406617x^{14}+756449132x^{13}+732355386x^{12}+562809398x^{11}\\ &+344991923x^{10}+169015680x^{9}+66108684x^{8}+20551670x^{7}\\ &+5033797x^{6}+957536x^{5}+138296x^{4}+14632x^{3}+1068x^{2}+48x+1.\end{aligned}$$

Hence, the number of independent sets of all possible sizes in the hexacyclic system has been fully delineated.

The following conclusion provides a computational formula for the Merrifield-Simmons index of a hexacyclic system.

Theorem 3.12. *For any hexacyclic system $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ with h hexagons, the Merrifield-Simmons index of $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ is given by*

$$\sigma(F_{\vartheta_1\vartheta_2\cdots\vartheta_h})=tr\Big(\prod_{i=1}^{h}\mathbf{H}_i\Big),$$

where $\mathbf{H}_i=\mathbf{X}$ if $\vartheta_i=\alpha$, $\mathbf{H}_i=\mathbf{Y}$ if $\vartheta_i=\beta$, $\mathbf{H}_i=\mathbf{Z}$ if $\vartheta_i=\gamma$, and

$$\mathbf{X}=\begin{pmatrix}3&2&2&1\\2&2&1&1\\2&1&2&1\\1&1&1&1\end{pmatrix},\mathbf{Y}=\begin{pmatrix}3&2&2&1\\3&0&2&0\\2&2&1&1\\2&0&1&0\end{pmatrix},\mathbf{Z}=\begin{pmatrix}3&2&2&1\\2&1&2&1\\3&2&0&0\\2&1&0&0\end{pmatrix}.$$

Proof. Since the Merrifield-Simmons index of a graph G can be obtained by $\sigma(G) = \Phi(G, 1)$, one can directly obtain the Merrifield-Simmons index in a hexacyclic system by plugging $x = 1$ into Theorem 3.10. ■

We next turn to studying the computation of the independence polynomial for the Möbius hexacyclic systems.

Theorem 3.13. *Let $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ be a hexacyclic system with h hexagons. The independence polynomial of its Möbius counterpart $M_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ is given by*

$$\Phi(M_{\vartheta_1\vartheta_2\cdots\vartheta_h}, x) = tr\bigg(\Big(\prod_{i=1}^{h}\mathbf{H}_i(x)\Big)\mathbf{E}_{(2,3)}\bigg),$$

where $\mathbf{E}_{(2,3)} = (\mathbf{e}_1, \mathbf{e}_3, \mathbf{e}_2, \mathbf{e}_4)$, $\mathbf{H}_i(x) = \mathbf{X}(x)$ *if* $\vartheta_i = \alpha$, $\mathbf{H}_i(x) = \mathbf{Y}(x)$ *if* $\vartheta_i = \beta$, $\mathbf{H}_i(x) = \mathbf{Z}(x)$ *if* $\vartheta_i = \gamma$.

Proof. Let $B_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ be the corresponding hexagonal chain created from the Möbius hexacyclic system $M_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ by cutting along the common edge u_0v_0, and the edge u_0v_0 is divided into two edges uv and $u'v'$, which appear in its corresponding hexagonal chain and $N(u') = \{v', q\}$ and $N(v') = \{u', p\}$. Similar to the proof of Theorem 3.10, we can get

$$\Phi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - p - q - u' - v', x) = \mathbf{e}_1^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{H}_i(x)\Big)\mathbf{e}_1,$$

$$x\Phi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - p - N[q] - v' - u, x) = \mathbf{e}_2^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{H}_i(x)\Big)\mathbf{e}_3,$$

$$x\Phi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - N[p] - q - u' - v, x) = \mathbf{e}_3^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{H}_i(x)\Big)\mathbf{e}_2,$$

$$x^2\Phi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - N[p] - N[q] - u - v, x) = \mathbf{e}_4^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{H}_i(x)\Big)\mathbf{e}_4,$$

where $\mathbf{H}_i(x) = \mathbf{X}(x)$ if $\vartheta_i = \alpha$, $\mathbf{H}_i(x) = \mathbf{Y}(x)$ if $\vartheta_i = \beta$, $\mathbf{H}_i(x) = \mathbf{Z}(x)$ if $\vartheta_i = \gamma$.

Then, using Lemma 2.2, we have

$$\begin{aligned}
\Phi(M_{\vartheta_1\vartheta_2\cdots\vartheta_h}, x) =& \Phi(M_{\vartheta_1\vartheta_2\cdots\vartheta_h} - p, x) + x\Phi(M_{\vartheta_1\vartheta_2\cdots\vartheta_h} - N[p], x)\\
=& \Phi(M_{\vartheta_1\vartheta_2\cdots\vartheta_h} - p - q, x) + x\Phi(M_{\vartheta_1\vartheta_2\cdots\vartheta_h} - p - N[q], x)\\
&+ x\Phi(M_{\vartheta_1\vartheta_2\cdots\vartheta_h} - N[p] - q, x) + x^2\Phi(M_{\vartheta_1\vartheta_2\cdots\vartheta_h} - N[p] - N[q], x)\\
=& \Phi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - p - q - v' - u', x) + x\Phi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - p - N[q] - v' - u, x)\\
&+ x\Phi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - N[p] - q - u' - v, x)\\
&+ x^2\Phi(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - N[p] - N[q] - u - v, x)\\
=& \mathbf{e}_1^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{H}_i(x)\Big)\mathbf{e}_1 + \mathbf{e}_2^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{H}_i(x)\Big)\mathbf{e}_3\\
&+ \mathbf{e}_3^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{H}_i(x)\Big)\mathbf{e}_2 + \mathbf{e}_4^{\mathrm{T}}\Big(\prod_{i=1}^{h}\mathbf{H}_i(x)\Big)\mathbf{e}_4\\
=& tr\bigg(\Big(\prod_{i=1}^{h}\mathbf{H}_i(x)\Big)\mathbf{E}_{(2,3)}\bigg).
\end{aligned}$$

Therefore, we arrive at the desired result. ■

The following example illustrates that the independence polynomial of the Möbius hexacyclic system depicted in Figure 2 can be derived by using Theorem 3.13.

Example 3.14. For the Möbius hexacyclic system $G = M_{\alpha\beta\alpha\beta\beta\gamma\beta\beta\beta\gamma\beta\beta}$ as shown in Figure 2, applying Theorem 3.13, we can get

$$\begin{aligned}\Phi(G,x) = &\, tr\big(\mathbf{X}(x)\mathbf{Y}(x)\mathbf{X}(x)\mathbf{Y}(x)^2\mathbf{Z}(x)\mathbf{Y}(x)^3\mathbf{Z}(x)\mathbf{Y}(x)^2\mathbf{E}_{(2,3)}\big)\\ =&\, 71x^{23} + 2436x^{22} + 43838x^{21} + 490875x^{20} + 3652378x^{19} + 18834754x^{18}\\ &+ 69627907x^{17} + 189734075x^{16} + 389871299x^{15} + 615229035x^{14}\\ &+ 756341032x^{13} + 732309243x^{12} + 562795631x^{11} + 344989114x^{10}\\ &+ 169015307x^{9} + 66108655x^{8} + 20551669x^{7} + 5033797x^{6} + 957536x^{5}\\ &+ 138296x^{4} + 14632x^{3} + 1068x^{2} + 48x + 1.\end{aligned}$$

Theorem 3.15. *For any hexacyclic system $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ with h hexagons, the Merrifield-Simmons index of its Möbius counterpart $M_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ is given by*

$$\sigma(M_{\vartheta_1\vartheta_2\cdots\vartheta_h}) = tr\bigg(\Big(\prod_{i=1}^{h}\mathbf{H}_i\Big)\mathbf{E}_{(2,3)}\bigg),$$

where $\mathbf{E}_{(2,3)} = (\mathbf{e}_1, \mathbf{e}_3, \mathbf{e}_2, \mathbf{e}_4)$, $\mathbf{H}_i = \mathbf{X}$ if $\vartheta_i = \alpha$, $\mathbf{H}_i = \mathbf{Y}$ if $\vartheta_i = \beta$, $\mathbf{H}_i = \mathbf{Z}$ if $\vartheta_i = \gamma$, and

$$\mathbf{X} = \begin{pmatrix} 3 & 2 & 2 & 1\\ 2 & 2 & 1 & 1\\ 2 & 1 & 2 & 1\\ 1 & 1 & 1 & 1\end{pmatrix}, \mathbf{Y} = \begin{pmatrix} 3 & 2 & 2 & 1\\ 3 & 0 & 2 & 0\\ 2 & 2 & 1 & 1\\ 2 & 0 & 1 & 0\end{pmatrix}, \mathbf{Z} = \begin{pmatrix} 3 & 2 & 2 & 1\\ 2 & 1 & 2 & 1\\ 3 & 2 & 0 & 0\\ 2 & 1 & 0 & 0\end{pmatrix}.$$

Proof. The result can be straightforwardly derived from Theorem 3.13 by substituting $x = 1$. ■

Explicit closed-form formulas for the Merrifield-Simmons index of the linear hexacyclic system $F_{\alpha\alpha\cdots\alpha}$ and its Möbius counterpart $M_{\alpha\alpha\cdots\alpha}$ are given below.

Corollary 3.16. *For a linear hexacyclic system $F_{\alpha\alpha\cdots\alpha}$ with $h \geq 3$ hexagons and its Möbius counterpart $M_{\alpha\alpha\cdots\alpha}$, we have $\sigma(F_{\alpha\alpha\cdots\alpha}) = \big(\frac{7+\sqrt{33}}{2}\big)^h + \big(\frac{7-\sqrt{33}}{2}\big)^h + 1$ and $\sigma(M_{\alpha\alpha\cdots\alpha}) = \big(\frac{7+\sqrt{33}}{2}\big)^h + \big(\frac{7-\sqrt{33}}{2}\big)^h - 1$.*

Proof. It is not difficult to verify that matrix $\mathbf{X}$ is similar to the diagonal matrix $\mathbf{\Lambda}$, i.e., $\mathbf{\Lambda} = \mathbf{U}^{-1}\mathbf{X}\mathbf{U}$, where

$$\mathbf{\Lambda} = \begin{pmatrix} 0 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & \frac{7-\sqrt{33}}{2} & 0\\ 0 & 0 & 0 & \frac{7+\sqrt{33}}{2}\end{pmatrix}, \mathbf{U} = \begin{pmatrix} 1 & 0 & \frac{3(5\sqrt{33}-29)}{7\sqrt{33}-39} & \frac{3(5\sqrt{33}+29)}{7\sqrt{33}+39}\\ -1 & -1 & \frac{11\sqrt{33}-63}{7\sqrt{33}-39} & \frac{11\sqrt{33}+63}{7\sqrt{33}+39}\\ -1 & 1 & \frac{11\sqrt{33}-63}{7\sqrt{33}-39} & \frac{11\sqrt{33}+63}{7\sqrt{33}+39}\\ 1 & 0 & 1 & 1\end{pmatrix}.$$

Then, by Theorems 3.12 and 3.15, we have

$$\sigma(F_{\alpha\alpha\cdots\alpha}) = tr\big(\mathbf{X}^h\big) = tr\big(\mathbf{\Lambda}^h\big) = \big(\tfrac{7+\sqrt{33}}{2}\big)^h + \big(\tfrac{7-\sqrt{33}}{2}\big)^h + 1,$$

and

$$\sigma(M_{\alpha\alpha\cdots\alpha}) = tr\big(\mathbf{X}^h\mathbf{E}_{(2,3)}\big) = tr\big(\mathbf{U}\mathbf{\Lambda}^h\mathbf{U}^{-1}\mathbf{E}_{(2,3)}\big) = \big(\tfrac{7+\sqrt{33}}{2}\big)^h + \big(\tfrac{7-\sqrt{33}}{2}\big)^h - 1.$$

This completes the proof. ■

Corollary 3.17. *For a helical hexacyclic system $F_{\beta\beta\dots\beta}$ with $h \geq 3$ hexagons and its Möbius counterpart $M_{\beta\dots\beta}$, we have $\sigma(F_{\beta\beta\dots\beta}) = tr\big(\mathbf{Y}^h\big)$ and $\sigma(M_{\beta\beta\dots\beta}) = tr\big(\mathbf{Y}^h\mathbf{E}_{(2,3)}\big)$.*

Corollary 3.18. *For a zig-zag hexacyclic system $F_{\beta\gamma\beta\gamma\dots}$ with $h \geq 3$ hexagons and its Möbius counterpart $M_{\beta\gamma\beta\gamma\dots}$, we have*

- $\sigma(F_{\beta\gamma\beta\gamma\dots}) = \begin{cases} \sigma(F_{\beta\gamma\beta\gamma\dots\beta\gamma}) = tr\big((\mathbf{YZ})^{\frac{h}{2}}\big), & \text{if } h \text{ is even,} \\ \sigma(F_{\beta\gamma\beta\gamma\dots\gamma\beta}) = tr\big((\mathbf{YZ})^{\frac{h-1}{2}}\mathbf{Y}\big), & \text{if } h \text{ is odd.} \end{cases}$
- $\sigma(M_{\beta\gamma\beta\gamma\dots}) = \begin{cases} \sigma(M_{\beta\gamma\beta\gamma\dots\beta\gamma}) = tr\big((\mathbf{YZ})^{\frac{h}{2}}\mathbf{E}_{(2,3)}\big), & \text{if } h \text{ is even,} \\ \sigma(M_{\beta\gamma\beta\gamma\dots\gamma\beta}) = tr\big((\mathbf{YZ})^{\frac{h-1}{2}}\mathbf{Y}\mathbf{E}_{(2,3)}\big), & \text{if } h \text{ is odd.} \end{cases}$

4 Concluding remarks

In this paper, we have successfully derived computational formulas for the matching polynomial and independence polynomial of both hexacyclic systems and Möbius hexacyclic systems through the utilization of the transfer matrix technique. We proved that the matching and independence polynomials of an arbitrary hexacyclic system $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ can each be expressed as the trace of the product of h matrices. Furthermore, we demonstrated that the matching and independence polynomials of any Möbius hexacyclic system $M_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ can be expressed as the trace of products of certain matrices, respectively. Therefore, for an arbitrary hexacyclic system and its Möbius counterpart, the number of matchings of any given size and the number of independent sets of any given size can all be obtained by solving their matching polynomials and independence polynomials. As applications, computational formulas for the Hosoya index and Merrifield-Simmons index of both arbitrary hexacyclic systems and Möbius hexacyclic systems are also obtained.
Two graphs G and H are matching equivalent if their matching polynomials are identical. Similarly, two graphs are independence equivalent if their independence polynomials coincide. Based on the established formulas in Theorems 3.1, 3.4, 3.10 and 3.13, we calculated the matching and independence polynomials for all non-isomorphic hexacyclic systems of length 5 and of length 6 and their Möbius counterparts, and found some matching equivalent graphs and independence equivalent graphs. Furthermore, certain Möbius hexacyclic systems are found to be both matching equivalent and independence equivalent. This phenomenon is absent in hexagonal chains, indicating that cylindrical configurations and Möbius configurations exert a distinct influence on the distribution of matchings and independent sets. The matching polynomials and independence polynomials for these matching equivalent or independence equivalent graphs are given in Appendix.

By applying Theorems 3.3, 3.6, 3.12 and 3.15, the Hosoya indices and Merrifield-Simmons indices for non-isomorphic hexacyclic systems of length 5 and of length 6, along with their Möbius counterparts, are presented in Tables 1 and 2, respectively. Through a careful analysis of these numerical results, we propose the following conjectures for further study.

Conjecture 4.1. *Among all hexacyclic systems (Möbius hexacyclic systems) with $h \geq 7$ hexagons, the linear hexacyclic system $F_{\alpha\alpha\dots\alpha}$ ($M_{\alpha\alpha\dots\alpha}$) attains the minimum z-index and the zig-zag hexacyclic system $F_{\beta\gamma\beta\gamma\dots}$ ($M_{\beta\gamma\beta\gamma\dots}$) attains the maximum z-index, respectively.*

Conjecture 4.2. *Among all hexacyclic systems (Möbius hexacyclic systems) with $h \geq 7$ hexagons, the linear hexacyclic system $F_{\alpha\alpha\dots\alpha}$ ($M_{\alpha\alpha\dots\alpha}$) attains the maximum σ-index and the zig-zag hexacyclic system $F_{\beta\gamma\beta\gamma\dots}$ ($M_{\beta\gamma\beta\gamma\dots}$) attains the minimum σ-index, respectively.*

Table 1: The Hosoya indices and Merrifield-Simmons indices for non-isomorphic hexacyclic systems of length 5 and their Möbius counterparts.

Hexacyclic system	z-index	σ-index	Hexacyclic system	z-index	σ-index
$F_{\alpha\alpha\alpha\alpha\alpha}$	36110	10508	$M_{\alpha\alpha\alpha\alpha\alpha}$	36108	10506
$F_{\beta\beta\beta\beta\beta}$	39646	9874	$M_{\beta\beta\beta\beta\beta}$	39765	9916
$F_{\alpha\alpha\alpha\alpha\beta}$	36988	10345	$M_{\alpha\alpha\alpha\alpha\beta}$	36991	10348
$F_{\alpha\beta\beta\beta\beta}$	39122	10018	$M_{\alpha\beta\beta\beta\beta}$	39100	9991
$F_{\beta\gamma\gamma\gamma\gamma}$	39818	9877	$M_{\beta\gamma\gamma\gamma\gamma}$	39765	9916
$F_{\alpha\alpha\beta\beta\beta}$	38376	10108	$M_{\alpha\alpha\beta\beta\beta}$	38390	10120
$F_{\beta\beta\alpha\alpha\alpha}$	37658	10240	$M_{\beta\beta\alpha\alpha\alpha}$	37652	10234
$F_{\beta\alpha\beta\alpha\alpha}$	37872	10198	$M_{\beta\alpha\beta\alpha\alpha}$	37868	10192
$F_{\beta\beta\gamma\gamma\gamma}$	39800	9886	$M_{\beta\beta\gamma\gamma\gamma}$	39765	9916
$F_{\beta\gamma\beta\gamma\beta}$	39978	9853	$M_{\beta\gamma\beta\gamma\beta}$	40094	9832
$F_{\alpha\alpha\alpha\beta\gamma}$	37764	10213	$M_{\alpha\alpha\alpha\beta\gamma}$	37761	10210
$F_{\alpha\alpha\beta\alpha\gamma}$	37885	10192	$M_{\alpha\alpha\beta\alpha\gamma}$	37880	10189
$F_{\beta\beta\beta\alpha\gamma}$	39195	9988	$M_{\beta\beta\beta\alpha\gamma}$	39100	9991
$F_{\beta\beta\alpha\beta\gamma}$	39254	9976	$M_{\beta\beta\alpha\beta\gamma}$	39175	9979
$F_{\alpha\beta\beta\gamma\gamma}$	39155	9997	$M_{\alpha\beta\beta\gamma\gamma}$	39141	9988
$F_{\alpha\beta\gamma\beta\gamma}$	39372	9946	$M_{\alpha\beta\gamma\beta\gamma}$	39355	9946
$F_{\alpha\beta\gamma\gamma\beta}$	39252	9976	$M_{\alpha\beta\gamma\gamma\beta}$	39260	9967
$F_{\beta\alpha\alpha\gamma\gamma}$	38451	10099	$M_{\beta\alpha\alpha\gamma\gamma}$	38390	10120
$F_{\beta\alpha\gamma\alpha\gamma}$	38653	10060	$M_{\beta\alpha\gamma\alpha\gamma}$	38552	10090
$F_{\beta\alpha\gamma\gamma\alpha}$	38554	10081	$M_{\beta\alpha\gamma\gamma\alpha}$	38552	10090
$F_{\beta\gamma\alpha\alpha\gamma}$	38558	10075	$M_{\beta\gamma\alpha\alpha\gamma}$	38455	10105

Appendix

1. The independence polynomials for independence equivalent but not matching equivalent (Möbius) hexacyclic systems of length 5 or 6

$\Phi(F_{\beta\beta\alpha\beta\gamma}, x) = \Phi(F_{\alpha\beta\gamma\gamma\beta}, x) = 2x^{10} + 34x^9 + 320x^8 + 1298x^7 + 2615x^6 + 2905x^5 + 1886x^4 + 730x^3 + 165x^2 + 20x + 1,$

$\Phi(F_{\alpha\gamma\gamma\beta\gamma\gamma}, x) = \Phi(F_{\alpha\gamma\beta\beta\gamma\gamma}, x) = 35x^{11} + 502x^{10} + 2958x^9 + 8968x^8 + 15627x^7 + 16703x^6 + 11368x^5 + 5002x^4 + 1412x^3 + 246x^2 + 24x + 1,$

$\Phi(F_{\alpha\beta\gamma\alpha\gamma\gamma}, x) = \Phi(F_{\alpha\beta\alpha\beta\gamma\gamma}, x) = 2x^{12} + 42x^{11} + 535x^{10} + 3073x^9 + 9162x^8 + 15785x^7 + 16768x^6 + 11381x^5 + 5003x^4 + 1412x^3 + 246x^2 + 24x + 1,$

$\Phi(F_{\alpha\beta\gamma\beta\gamma\gamma}, x) = \Phi(F_{\alpha\beta\gamma\gamma\beta\gamma}, x) = 37x^{11} + 495x^{10} + 2914x^9 + 8906x^8 + 15590x^7 + 16693x^6 + 11367x^5 + 5002x^4 + 1412x^3 + 246x^2 + 24x + 1,$

$\Phi(F_{\alpha\gamma\gamma\beta\gamma\gamma}, x) = \Phi(F_{\alpha\gamma\beta\beta\gamma\gamma}, x) = 35x^{11} + 502x^{10} + 2958x^9 + 8968x^8 + 15627x^7 + 16703x^6 + 11368x^5 + 5002x^4 + 1412x^3 + 246x^2 + 24x + 1,$

$\Phi(F_{\alpha\beta\gamma\beta\gamma\gamma}, x) = \Phi(F_{\alpha\beta\gamma\gamma\beta\gamma}, x) = 37x^{11} + 495x^{10} + 2914x^9 + 8906x^8 + 15590x^7 + 16693x^6 + 11367x^5 + 5002x^4 + 1412x^3 + 246x^2 + 24x + 1,$

$\Phi(F_{\alpha\beta\gamma\alpha\gamma\gamma}, x) = \Phi(F_{\alpha\beta\alpha\beta\gamma\gamma}, x) = 2x^{12} + 42x^{11} + 535x^{10} + 3073x^9 + 9162x^8 + 15785x^7 + 16768x^6 + 11381x^5 + 5003x^4 + 1412x^3 + 246x^2 + 24x + 1,$

$\Phi(F_{\alpha\alpha\beta\alpha\alpha\beta}, x) = \Phi(F_{\alpha\alpha\alpha\beta\alpha\gamma}, x) = 2x^{12} + 50x^{11} + 637x^{10} + 3418x^9 + 9668x^8 + 16156x^7 + 16910x^6 + 11408x^5 + 5005x^4 + 1412x^3 + 246x^2 + 24x + 1,$

Table 2: The Hosoya indices and Merrifield-Simmons indices for non-isomorphic hexacyclic systems of length 6 and their Möbius counterparts.

Hexacyclic system	z-index	σ-index	Hexacyclic system	z-index	σ-index
$F_{\alpha\alpha\alpha\alpha\alpha\alpha}$	294536	66954	$M_{\alpha\alpha\alpha\alpha\alpha\alpha}$	294534	66952
$F_{\beta\beta\beta\beta\beta\beta}$	330092	62507	$M_{\beta\beta\beta\beta\beta\beta}$	330422	62333
$F_{\alpha\alpha\alpha\alpha\alpha\beta}$	301718	65930	$M_{\alpha\alpha\alpha\alpha\alpha\beta}$	301721	65933
$F_{\alpha\alpha\alpha\alpha\beta\beta}$	307146	65234	$M_{\alpha\alpha\alpha\alpha\beta\beta}$	307140	65228
$F_{\alpha\alpha\alpha\beta\alpha\beta}$	308906	64964	$M_{\alpha\alpha\alpha\beta\alpha\beta}$	308902	64958
$F_{\alpha\alpha\beta\alpha\alpha\beta}$	309050	64937	$M_{\alpha\alpha\beta\alpha\alpha\beta}$	309058	64928
$F_{\alpha\alpha\alpha\beta\beta\beta}$	313097	64448	$M_{\alpha\alpha\alpha\beta\beta\beta}$	313111	64460
$F_{\alpha\alpha\beta\beta\alpha\beta}$	314480	64256	$M_{\alpha\alpha\beta\beta\alpha\beta}$	314500	64265
$F_{\alpha\beta\alpha\beta\alpha\beta}$	316086	64028	$M_{\alpha\beta\alpha\beta\alpha\beta}$	316199	64016
$F_{\alpha\alpha\beta\beta\beta\beta}$	319076	63731	$M_{\alpha\alpha\beta\beta\beta\beta}$	319054	63704
$F_{\alpha\beta\alpha\beta\beta\beta}$	320465	63539	$M_{\alpha\beta\alpha\beta\beta\beta}$	320518	63500
$F_{\alpha\beta\beta\alpha\beta\beta}$	320094	63602	$M_{\alpha\beta\beta\alpha\beta\beta}$	320113	63572
$F_{\alpha\beta\beta\beta\beta\beta}$	325011	62960	$M_{\alpha\beta\beta\beta\beta\beta}$	325130	63002
$F_{\beta\gamma\gamma\gamma\gamma\gamma}$	331109	62285	$M_{\beta\gamma\gamma\gamma\gamma\gamma}$	330422	62333
$F_{\beta\beta\gamma\gamma\gamma\gamma}$	330884	62321	$M_{\beta\beta\gamma\gamma\gamma\gamma}$	330422	62333
$F_{\beta\gamma\beta\gamma\gamma\gamma}$	332421	62063	$M_{\beta\gamma\beta\gamma\gamma\gamma}$	331730	62156
$F_{\beta\gamma\gamma\beta\gamma\gamma}$	332098	62135	$M_{\beta\gamma\gamma\beta\gamma\gamma}$	331515	62201
$F_{\beta\beta\beta\gamma\gamma\gamma}$	330948	62303	$M_{\beta\beta\beta\gamma\gamma\gamma}$	330422	62333
$F_{\beta\beta\gamma\beta\gamma\gamma}$	332124	62126	$M_{\beta\beta\gamma\beta\gamma\gamma}$	331730	62156
$F_{\beta\gamma\beta\gamma\beta\gamma}$	333947	61814	$M_{\beta\gamma\beta\gamma\beta\gamma}$	333010	61970
$F_{\alpha\beta\gamma\gamma\gamma\gamma}$	325751	62873	$M_{\alpha\beta\gamma\gamma\gamma\gamma}$	325698	62912
$F_{\alpha\gamma\beta\gamma\gamma\gamma}$	326335	62783	$M_{\alpha\gamma\beta\gamma\gamma\gamma}$	326430	62780
$F_{\alpha\gamma\gamma\beta\gamma\gamma}$	326024	62846	$M_{\alpha\gamma\gamma\beta\gamma\gamma}$	326083	62852
$F_{\alpha\beta\beta\gamma\gamma\gamma}$	325524	62918	$M_{\alpha\beta\beta\gamma\gamma\gamma}$	325489	62948
$F_{\alpha\beta\gamma\beta\gamma\gamma}$	326995	62687	$M_{\alpha\beta\gamma\beta\gamma\gamma}$	326930	62708
$F_{\alpha\beta\gamma\gamma\beta\gamma}$	327019	62687	$M_{\alpha\beta\gamma\gamma\beta\gamma}$	326918	62717
$F_{\alpha\gamma\beta\beta\gamma\gamma}$	326056	62846	$M_{\alpha\gamma\beta\beta\gamma\gamma}$	326133	62843
$F_{\alpha\gamma\beta\gamma\beta\gamma}$	327816	62552	$M_{\alpha\gamma\beta\gamma\beta\gamma}$	327932	62531
$F_{\alpha\alpha\beta\gamma\gamma\gamma}$	319733	63611	$M_{\alpha\alpha\beta\gamma\gamma\gamma}$	319713	63602
$F_{\alpha\beta\alpha\gamma\gamma\gamma}$	320613	63497	$M_{\alpha\beta\alpha\gamma\gamma\gamma}$	320518	63500
$F_{\alpha\alpha\gamma\beta\gamma\gamma}$	320280	63527	$M_{\alpha\alpha\gamma\beta\gamma\gamma}$	320282	63518
$F_{\alpha\beta\gamma\alpha\gamma\gamma}$	321019	63434	$M_{\alpha\beta\gamma\alpha\gamma\gamma}$	320940	63437
$F_{\alpha\gamma\alpha\beta\gamma\gamma}$	321113	63425	$M_{\alpha\gamma\alpha\beta\gamma\gamma}$	321178	63404
$F_{\alpha\alpha\beta\beta\gamma\gamma}$	319420	63674	$M_{\alpha\alpha\beta\beta\gamma\gamma}$	319406	63665
$F_{\alpha\alpha\beta\gamma\beta\gamma}$	321195	63362	$M_{\alpha\alpha\beta\gamma\beta\gamma}$	321178	63362
$F_{\alpha\beta\alpha\beta\gamma\gamma}$	321077	63434	$M_{\alpha\beta\alpha\beta\gamma\gamma}$	321000	63437
$F_{\alpha\beta\alpha\gamma\beta\gamma}$	322091	63248	$M_{\alpha\beta\alpha\gamma\beta\gamma}$	321975	63269
$F_{\alpha\beta\gamma\alpha\beta\gamma}$	322017	63257	$M_{\alpha\beta\gamma\alpha\beta\gamma}$	321905	63278
$F_{\alpha\beta\gamma\alpha\gamma\beta}$	321802	63308	$M_{\alpha\beta\gamma\alpha\gamma\beta}$	321905	63278
$F_{\alpha\alpha\alpha\beta\gamma\gamma}$	313660	64367	$M_{\alpha\alpha\alpha\beta\gamma\gamma}$	313664	64373
$F_{\alpha\alpha\beta\alpha\gamma\gamma}$	314561	64244	$M_{\alpha\alpha\beta\alpha\gamma\gamma}$	314559	64253
$F_{\alpha\alpha\beta\gamma\alpha\gamma}$	315362	64109	$M_{\alpha\alpha\beta\gamma\alpha\gamma}$	315354	64118
$F_{\alpha\beta\alpha\gamma\alpha\gamma}$	316300	63986	$M_{\alpha\beta\alpha\gamma\alpha\gamma}$	316199	64016
$F_{\alpha\beta\gamma\alpha\alpha\gamma}$	315457	64088	$M_{\alpha\beta\gamma\alpha\alpha\gamma}$	315354	64118
$F_{\alpha\alpha\alpha\alpha\beta\gamma}$	308025	65072	$M_{\alpha\alpha\alpha\alpha\beta\gamma}$	308022	65069
$F_{\alpha\alpha\alpha\beta\alpha\gamma}$	309014	64937	$M_{\alpha\alpha\alpha\beta\alpha\gamma}$	309009	64934
$F_{\alpha\alpha\beta\alpha\alpha\gamma}$	309075	64928	$M_{\alpha\alpha\beta\alpha\alpha\gamma}$	309058	64928

$\Phi(M_{\alpha\beta\gamma\alpha\gamma\gamma}, x) = \Phi(M_{\alpha\beta\alpha\beta\gamma\gamma}, x) = 37x^{11}+533x^{10}+3079x^9+9167x^8+15786x^7+16768x^6+11381x^5 + 5003x^4 + 1412x^3 + 246x^2 + 24x + 1.$

2. The matching polynomials and independence polynomials for matching equivalent and independence equivalent Möbius hexacyclic systems of length 5 or 6

$\Psi(M_{\alpha\beta\beta\beta\beta}, x) = \Psi(M_{\beta\beta\beta\alpha\gamma}, x) = 10x^{10} + 371x^9 + 2713x^8 + 7912x^7 + 11698x^6 + 9779x^5 + 4867x^4 + 1464x^3 + 260x^2 + 25x + 1,$

$\Phi(M_{\alpha\beta\beta\beta\beta}, x) = \Phi(M_{\beta\beta\beta\alpha\gamma}, x) = 29x^9 + 318x^8 + 1310x^7 + 2625x^6 + 2907x^5 + 1886x^4 + 730x^3 + 165x^2 + 20x + 1,$

$\Psi(M_{\beta\beta\beta\beta\beta}, x) = \Psi(M_{\beta\beta\gamma\gamma\gamma}, x) = 13x^{10} + 403x^9 + 2843x^8 + 8138x^7 + 11883x^6 + 9853x^5 + 4881x^4 + 1465x^3 + 260x^2 + 25x + 1,$

$\Phi(M_{\beta\beta\beta\beta\beta}, x) = \Phi(M_{\beta\beta\gamma\gamma\gamma}, x) = 2x^{10} + 34x^9 + 308x^8 + 1276x^7 + 2597x^6 + 2898x^5 + 1885x^4 + 730x^3 + 165x^2 + 20x + 1,$

$\Psi(M_{\alpha\alpha\beta\beta\beta}, x) = \Psi(M_{\beta\alpha\alpha\gamma\gamma}, x) = 10x^{10} + 342x^9 + 2566x^8 + 7662x^7 + 11504x^6 + 9704x^5 + 4853x^4 + 1463x^3 + 260x^2 + 25x + 1,$

$\Phi(M_{\alpha\alpha\beta\beta\beta}, x) = \Phi(M_{\beta\alpha\alpha\gamma\gamma}, x) = 2x^{10} + 38x^9 + 350x^8 + 1356x^7 + 2655x^6 + 2916x^5 + 1887x^4 + 730x^3 + 165x^2 + 20x + 1,$

$\Psi(M_{\beta\alpha\gamma\alpha\gamma}, x) = \Psi(M_{\beta\alpha\gamma\gamma\alpha}, x) = 11x^{10} + 355x^9 + 2609x^8 + 7720x^7 + 11540x^6 + 9714x^5 + 4854x^4 + 1463x^3 + 260x^2 + 25x + 1,$

$\Phi(M_{\beta\alpha\gamma\alpha\gamma}, x) = \Phi(M_{\beta\alpha\gamma\gamma\alpha}, x) = 2x^{10} + 36x^9 + 341x^8 + 1344x^7 + 2649x^6 + 2915x^5 + 1887x^4 + 730x^3 + 165x^2 + 20x + 1,$

$\Psi(M_{\beta\gamma\beta\gamma\gamma\gamma}, x) = \Psi(M_{\beta\beta\gamma\beta\gamma\gamma}, x) = 18x^{12} + 804x^{11} + 8043x^{10} + 33247x^9 + 71838x^8 + 91301x^7 + 72796x^6 + 37661x^5 + 12786x^4 + 2818x^3 + 387x^2 + 30x + 1,$

$\Phi(M_{\beta\gamma\beta\gamma\gamma\gamma}, x) = \Phi(M_{\beta\beta\gamma\beta\gamma\gamma}, x) = 33x^{11}+463x^{10}+2801x^9+8731x^8+15453x^7+16636x^6+11355x^5 + 5001x^4 + 1412x^3 + 246x^2 + 24x + 1,$

$\Psi(M_{\alpha\beta\alpha\beta\beta\beta}, x) = \Psi(M_{\alpha\beta\alpha\gamma\gamma\gamma}, x) = 15x^{12} + 707x^{11} + 7272x^{10} + 30860x^9 + 68289x^8 + 88487x^7 + 71552x^6 + 37355x^5 + 12747x^4 + 2816x^3 + 387x^2 + 30x + 1,$

$\Phi(M_{\alpha\beta\alpha\beta\beta\beta}, x) = \Phi(M_{\alpha\beta\alpha\gamma\gamma\gamma}, x) = 37x^{11}+527x^{10}+3082x^9+9196x^8+15813x^7+16777x^6+11382x^5 + 5003x^4 + 1412x^3 + 246x^2 + 24x + 1,$

$\Psi(M_{\alpha\beta\gamma\alpha\beta\gamma}, x) = \Psi(M_{\alpha\beta\gamma\alpha\gamma\beta}, x) = 14x^{12} + 700x^{11} + 7308x^{10} + 31126x^9 + 68788x^8 + 88892x^7 + 71710x^6 + 37384x^5 + 12749x^4 + 2816x^3 + 387x^2 + 30x + 1,$

$\Phi(M_{\alpha\beta\gamma\alpha\beta\gamma}, x) = \Phi(M_{\alpha\beta\gamma\alpha\gamma\beta}, x) = 39x^{11}+526x^{10}+3035x^9+9105x^8+15749x^7+16758x^6+11380x^5 + 5003x^4 + 1412x^3 + 246x^2 + 24x + 1,$

$\Psi(M_{\alpha\alpha\beta\gamma\alpha\gamma}, x) = \Psi(M_{\alpha\beta\gamma\alpha\alpha\gamma}, x) = 14x^{12} + 635x^{11} + 6799x^{10} + 29651x^9 + 66715x^8 + 87318x^7 + 71037x^6 + 37223x^5 + 12729x^4 + 2815x^3 + 387x^2 + 30x + 1,$

$\Phi(M_{\alpha\alpha\beta\gamma\alpha\gamma}, x) = \Phi(M_{\alpha\beta\gamma\alpha\alpha\gamma}, x) = 2x^{12} + 46x^{11} + 583x^{10} + 3230x^9 + 9389x^8 + 15953x^7 + 16834x^6 + 11394x^5 + 5004x^4 + 1412x^3 + 246x^2 + 24x + 1,$

$\Psi(M_{\alpha\alpha\beta\alpha\alpha\beta}, x) = \Psi(M_{\alpha\alpha\beta\alpha\alpha\gamma}, x) = 11x^{12} + 579x^{11} + 6349x^{10} + 28275x^9 + 64711x^8 + 85764x^7 + 70366x^6 + 37062x^5 + 12709x^4 + 2814x^3 + 387x^2 + 30x + 1,$

$\Phi(M_{\alpha\alpha\beta\alpha\alpha\beta}, x) = \Phi(M_{\alpha\alpha\beta\alpha\alpha\gamma}, x) = 47x^{11} + 634x^{10} + 3417x^9 + 9668x^8 + 16156x^7 + 16910x^6 + 11408x^5 + 5005x^4 + 1412x^3 + 246x^2 + 24x + 1,$

$\Psi(M_{\beta\beta\beta\beta\beta\beta}, x) = \Psi(M_{\beta\gamma\gamma\gamma\gamma\gamma}, x) = \Psi(M_{\beta\beta\gamma\gamma\gamma\gamma}, x) = \Psi(M_{\beta\beta\beta\gamma\gamma\gamma}, x) = 18x^{12} + 800x^{11} + 7988x^{10} + 32996x^9 + 71388x^8 + 90931x^7 + 72648x^6 + 37633x^5 + 12784x^4 + 2818x^3 + 387x^2 + 30x + 1,$

$\Phi(M_{\beta\beta\beta\beta\beta\beta}, x) = \Phi(M_{\beta\gamma\gamma\gamma\gamma\gamma}, x) = \Phi(M_{\beta\beta\gamma\gamma\gamma\gamma}, x) = \Phi(M_{\beta\beta\beta\gamma\gamma\gamma}, x) = 2x^{10} + 34x^9 + 308x^8 + 1276x^7 + 2597x^6 + 2898x^5 + 1885x^4 + 730x^3 + 165x^2 + 20x + 1.$

Conflicts of Interest. The author declares that he has no conflicts of interest regarding the publication of this article.

Acknowledgement. This work was supported by the National Natural Science Foundation of China (12201634), the Natural Science Foundation of Hunan Province (2023JJ30070) and the Education Department Foundation of Hunan Province(22B0828).

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