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The Maximal Matching Polynomial of Hexacyclic Systems

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Abstract

Hexacyclic systems have extensive applications in chemistry, combinatorics, and materials science, especially in the characterization of molecular structures and network topologies. The maximal matching polynomial is a fundamental graph invariant that encodes crucial structural and combinatorial information of graphs, which plays a key role in studying the matching properties and structural stability of graphs. In this study, we derive a general computational formula for the maximal matching polynomial of hexacyclic systems, which can be efficiently applied to any hexacyclic structure composed of hexagonal rings. Consequently, a computational formula for the number of maximal matchings of an arbitrary hexacyclic system can be derived. Furthermore, we prove that among all hexacyclic systems with the same length, the linear hexacyclic system has the minimum saturation number.

1 Introduction

All graphs considered throughout this paper are finite and simple. For a graph G, we denote its vertex set and edge set by $V(G)$ and $E(G)$, re-

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spectively. For a vertex $v \in V(G)$, its open neighborhood $N_G(v)$ consists of all vertices adjacent to v, while the closed neighborhood $N_G[v]$ includes v together with all its neighbors. Whenever the underlying graph is unambiguous, we write $N(v)$ and $N[v]$ for brevity. The degree of a vertex $v \in V(G)$ is defined as $d_G(v) = |N_G(v)|$. For any vertex $v \in V(G)$, $G - v$ denotes the graph derived by removing vertex v and all its incident edges from G. Analogously, for two distinct vertices $u, v \in V(G)$, $G-u-v$ refers to the graph obtained by deleting both vertices u and v along with their incident edges. We use P_n and C_n to denote the path and cycle graph of order n, respectively. The distance $d_G(u, v)$ between two vertices u and v in G is defined as the number of edges in a shortest path connecting u and v; we simply write $d(u, v)$ if G is clear from the context. Let $\mathbf{M}$ be a square matrix. We use $\mathsf{tr}(\mathbf{M})$ to represent its trace, and let $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$, $\mathbf{e}_4$, $\mathbf{e}_5$, $\mathbf{e}_6$, $\mathbf{e}_7$, $\mathbf{e}_8$, $\mathbf{e}_9$ denote the standard basis vectors in $\mathbb{R}^9$.

A matching is a set of edges without shared vertices, meaning no two edges in the set are adjacent, forming a collection of independent edges. A vertex $v \in V(G)$ is said to be saturated with respect to a matching $M \subseteq E(G)$ if there exists an edge $e \in M$ incident to v; otherwise, it is unsaturated. A maximal matching is a matching that cannot be extended by adding another edge from the graph–it is maximal under set inclusion, though it may not include the largest possible number of edges. A maximum matching is a maximal matching of maximum cardinality. The matching number $\mu(G)$ of a graph G is the cardinality of a maximum matching. A perfect matching is a special matching that covers every vertex of the graph, such that each vertex is incident to exactly one edge in the matching, existing only when the graph has an even number of vertices and satisfies certain structural conditions. In chemical graph theory, a perfect matching corresponds to a Kekulé structure, and the enumeration of Kekulé structures plays a pivotal role in the study of benzenoid hydrocarbons. The saturation number $s(G)$ of a graph G is defined as the minimum number of edges contained in any maximal matching of the graph, representing the smallest size a maximal matching can reach, which reflects the edge-saturation property of the graph under maximal matching constraints. For any graph G, the relationship between its matching

number and saturation number satisfies $\frac{\mu(G)}{2} \leq s(G) \leq \mu(G)$.

Let $\mathcal{K}$ denote the set of all maximal matchings in a graph G. The maximal matching polynomial of a graph was first introduced by Došlić and Zubac [7] in 2016. For a graph G, it is defined as

$$Z(G, x) = \sum_{K \in \mathcal{K}} x^{|K|} = \sum_{k \geq s(G)} m_k(G) x^k,$$

where $m_k(G)$ denotes the number of maximal matchings of size k in graph G. The total number of maximal matchings of a graph G is defined as $\zeta(G) = |\mathcal{K}| = \sum_{k \geq s(G)} m_k(G)$. The maximal matching polynomial evaluated at $x = 1$ coincides with the number of maximal matchings of G, i.e., $\zeta(G) = Z(G, 1)$. As a carrier of important information such as the number of perfect matchings (Kekulé structures), the saturation number, and the number of maximal matchings, investigating the computation and related properties of maximal matching polynomials is both interesting and significant. Recent research on the maximal matching and maximal matching polynomial can be found in [2, 5–7, 9, 14].

Coronoid hydrocarbons can be modeled as simple graphs known as coronoid systems. Notably, coronoid systems are rigorously defined within a planar regular hexagonal lattice. Let C' and C'' be two cycles embedded in this planar hexagonal lattice such that C'' lies strictly inside C'. A coronoid system is then defined as the induced graph formed by all vertices and edges situated on the outer perimeter C', on the inner perimeter C'', and in the region interior to C' but exterior to C''. As the most fundamental subclass of coronoid systems, a primitive coronoid system refers to a catacondensed coronoid without internal vertices. It consists of a single macrocyclic assembly of hexagons fused only via linear and angular junctions, and possesses a well-defined inner perimeter, outer perimeter, and central cavity, making it the simplest cyclic hexagonal structure containing an internal hole. A hollow hexagon is a subclass of primitive coronoid systems. It is characterized by exactly six outward-protruding corners and no inward-indented corners toward the central inner hole. Parameterized by six segment lengths, hollow hexagons correspond to kekulene and other related cycloarene molecules.

Hexacyclic systems are closed ring-like cyclic hexagonal structures, embedded either in a planar hexagonal lattice or on a cylindrical lattice. Specifically, only hexacyclic systems embedded in a planar regular hexagonal lattice satisfy the standard definitions of inner and outer perimeters. In contrast, for cylindrically embedded hexacyclic systems, the conventional inner and outer perimeters are reinterpreted as the top and bottom perimeters, respectively. Consider a hexacyclic system composed of h hexagons, where h is referred to as the system length. Such a system takes the form of a cyclic sequence of hexagons $C_6^{(1)}, C_6^{(2)}, \ldots, C_6^{(h)}$. Each hexagon shares exactly one edge with its two immediate neighbors, and no vertex is shared by more than two hexagons in the entire structure. For each $i \in \{1, 2, \ldots, h-1\}$, denote the common edge of $C_6^{(i)}$ and $C_6^{(i+1)}$ by $u_i v_i$; let $u_0 v_0$ denote the shared edge between $C_6^{(h)}$ and $C_6^{(1)}$. The vertices $u_0, u_1, \ldots, u_{h-1}$ lie on the inner (top) perimeter, while $v_0, v_1, \ldots, v_{h-1}$ lie on the outer (bottom) perimeter. Within $C_6^{(h)}$, the vertex neighborhoods are specified as $N(u_0) = \{p, v_0\}$ and $N(v_0) = \{q, u_0\}$. Taking all indices modulo h, each hexagon $C_6^{(i)}$ can be categorized by the shortest-path distances between consecutive perimeter vertices: an α-type if $d(u_{i-1}, u_i) = d(v_{i-1}, v_i) = 2$; a β-type if $d(u_{i-1}, u_i) = 1$ and $d(v_{i-1}, v_i) = 3$; a γ-type if $d(u_{i-1}, u_i) = 3$ and $d(v_{i-1}, v_i) = 1$. A general hexacyclic system is denoted as $F_{\vartheta_1 \vartheta_2 \cdots \vartheta_h}$ with $\vartheta_i \in \{\alpha, \beta, \gamma\}$. Representative configurations valid for arbitrary h include the uniform linear type $F_{\alpha\alpha\cdots\alpha}$, the helical type $F_{\beta\beta\cdots\beta}$, and the alternating zig-zag type $F_{\beta\gamma\beta\gamma\cdots}$. Cutting the cyclic shared edge $u_0 v_0$ in $F_{\vartheta_1 \vartheta_2 \cdots \vartheta_h}$ transforms the closed hexacyclic system into an open hexagonal chain $B_{\vartheta_1 \vartheta_2 \cdots \vartheta_h}$, where the original edge $u_0 v_0$ is split into two separate edges $uv \in E(C_6^{(1)})$ and $u'v' \in E(C_6^{(h)})$. Furthermore, the isomorphism relation $F_{\vartheta_1 \vartheta_2 \cdots \vartheta_h} \cong F_{\overline{\vartheta}_1 \overline{\vartheta}_2 \cdots \overline{\vartheta}_h}$ holds, where $\overline{\vartheta}_i = \alpha$ if $\vartheta_i = \alpha$; $\overline{\vartheta}_i = \gamma$ if $\vartheta_i = \beta$; $\overline{\vartheta}_i = \beta$ if $\vartheta_i = \gamma$. An illustrative example of a hexacyclic system and its corresponding open hexagonal chain is presented in Figure 1.

Based on the above definitions and classifications, coronoid systems (including primitive coronoid systems and hollow hexagons) are strictly confined to planar embeddings, whereas hexacyclic systems encompass both planar-embeddable and cylinder-embeddable subclasses. Consequ-

ently, both hollow hexagons and primitive coronoid systems fall within the planar-embeddable subclass of hexacyclic systems, which yields the strict hierarchical inclusion relation: Hollow hexagons $\subset$ Primitive coronoid systems $\subset$ Hexacyclic systems.

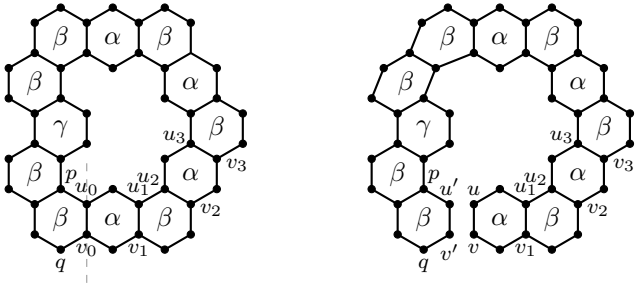

Figure 1. Hexacylic system $F_{\alpha\beta\alpha\beta\alpha\beta\alpha\beta\beta\gamma\beta\beta}$ and its corresponding hexagonal chain.

Recently, the problems of computing and extremizing important invariant parameters for coronoid systems, hexacyclic systems, primitive coronoid systems, and hollow hexagons have attracted considerable attention from researchers. For linear hexacyclic systems, the computation of several graph-spectrum-related parameters has been investigated in [8, 9, 11, 12]. Explicit expressions for a number of distance-based topological indices of circumcised donut benzenoid systems were derived in [1]. In [4], Cruz, Santamaría-Galvis and Rada determined the extremal values of several vertex-degree-based (VDB) topological indices over the families of primitive coronoid systems, catacondensed coronoid systems, and circumscribed coronoid systems. In [13], Oz *et al.* proposed a method based on the transfer matrix technique and the Hosoya vector to compute the Hosoya index of arbitrary primitive coronoid systems. In [10], Lopera and Cruz computed the Szeged index of hollow hexagons via the cut method. Using the same technique, Cruz and Santamaría-Galvis [3] obtained the Mostar index of hollow hexagons and established the extremal values of this index over the class of hollow hexagons with a fixed number of hexagons. Further investigating the computation and extremal properties of additional topological invariants over hexacyclic systems is therefore of both theoretical and practical importance.

In [2], Chen and Zhang derived formulas for the maximal matching polynomials of phenylene and benzenoid chains, thereby completely characterizing the number of maximal matchings of all sizes for such chains. However, as an important class of graphical models, the distribution of maximal matchings on hexacyclic systems remains unexplored–including the number of perfect matchings, the saturation number, and the number of minimum maximal matchings. In this paper, by extending the methodology developed in [2], we establish techniques to compute the maximal matching polynomial for an arbitrary hexacyclic system $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$. As a consequence, we derive a computational formula for the number of maximal matchings in any hexacyclic system. Furthermore, we prove that, among all hexacyclic systems of a fixed length, the linear hexacyclic system attains the minimum saturation number.

2 Main results

In this section, we first investigate methods for computing the maximal matching polynomial of hexacyclic systems and then determine the minimum saturation number among all hexacyclic systems of a given length.

Before presenting the main results, we introduce some technical lemmas and related definitions.

Lemma 2.1 ([2]). (i) *If $uv \in E(G)$ and $d_G(u) = 1$, then* $Z(G,x) = xZ(G-u-v,x) + x \sum_{w\in N_G(v)\setminus\{u\}} Z(G-u-v-w,x)$.

(ii) *For any graph G and vertex $v \in V(G)$ satisfying $N(v) = \{u,w\}$ and $uw \notin E(G)$, we have*

$$\begin{aligned} Z(G,x) =& xZ(G-u-v,x) + xZ(G-v-w,x) \\ &+ x^2 \sum_{\substack{s\in N_G(u)\setminus\{v\},\\ t\in N_G(w)\setminus\{v\}}} Z(G-u-w-s-t,x). \end{aligned}$$

(iii) *For a graph G with k components $R_1,\ldots,R_k$,* $Z(G,x) = \prod_{i=1}^{k} Z(R_i,x)$.

Definition 2.1 ([2]). Let G be a graph such that $\{pu, uv, vw\} \subseteq E(G)$ and $d_G(u) = d_G(v) = 2$. The vector $Z_{uv}(G, x)$ corresponding to the edge uv is given by $Z_{uv}(G, x) = (Z(G, x), Z(G - u, x), Z(G - v, x), Z(G - u - v, x), Z(G - p - u, x), Z(G - v - w, x), Z(G - N_G[u], x), Z(G - N_G[v], x), Z(G - N_G[u] - N_G[v], x))^\top$.

The following three matrices will be used in the subsequent discussion of this paper, as shown in Ref. [2].

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

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

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

Lemma 2.2 ([2]). *Let G be a graph obtained from the edge-coalescence of graph R and a hexagon, see* Figure 2. *Then* (i) $Z_{uv}(G, x) = \mathbf{A}(x)Z_{qr}(R, x)$, (ii) $Z_{uv}(G, x) = \mathbf{B}(x)Z_{pq}(R, x)$ *and* (iii) $Z_{uv}(G, x) =$

$\mathbf{C}(x)Z_{rw}(R,x)$.

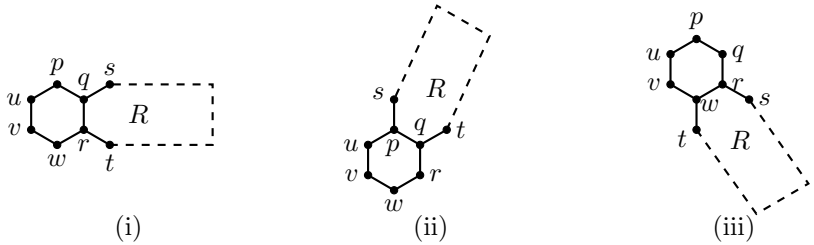

Figure 2. The graphs employed in Lemma 2.2.

For convenience, we occasionally denote the maximal matching polynomial of a graph G by $Z(G)$ and the vector $Z_{uv}(G,x)$ by $Z_{uv}(G)$, and resort to the notation $Z(G,x)$ and $Z_{uv}(G,x)$ when explicitly emphasizing the variable x.

We present the main results of this paper in what follows.

Theorem 2.1. *For any hexacyclic system $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ with h hexagons, the maximal matching polynomial of $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ is*

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

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 $C_6^{(1)}$, $C_6^{(2)}$, $\ldots$, $C_6^{(h)}$. 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. For $i\in\{1,2,3,\ldots,h\}$, we denote by $B_{\vartheta_i\vartheta_{i+1}\cdots\vartheta_h}$ the subchain of length $h-i+1$ composed of the sequence of hexagons $C_6^{(i)}$, $C_6^{(i+1)}$, $\ldots$, $C_6^{(h)}$, and define the functional matrix $\mathbf{M}_i(x)$ as: $\mathbf{M}_i(x)=\mathbf{A}(x)$ if $\vartheta_i=\alpha$; $\mathbf{M}_i(x)=\mathbf{B}(x)$ if $\vartheta_i=\beta$; $\mathbf{M}_i(x)=\mathbf{C}(x)$ if $\vartheta_i=\gamma$.

Note that $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}\cong F_{\overline{\vartheta}_1\overline{\vartheta}_2\cdots\overline{\vartheta}_h}$, where $\overline{\vartheta}_i=\alpha$ if $\vartheta_i=\alpha$; $\overline{\vartheta}_i=\gamma$ if $\vartheta_i=\beta$; $\overline{\vartheta}_i=\beta$ if $\vartheta_i=\gamma$. We need to consider the following five cases. A detailed derivation is provided only for the first case. The remaining cases

can be treated in a similar manner; therefore, the detailed computational verification steps are omitted.

Case 1: $\vartheta_{h-1} = \vartheta_h = \alpha$.

For a hexacyclic system $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ with $\vartheta_{h-1} = \vartheta_h = \alpha$, assume that $N(u_0) = \{p, s, v_0\}$, $N(v_0) = \{q, t, u_0\}$, $N(u_0) \cap N(u_{h-1}) = \{p\}$, $N(v_0) \cap N(v_{h-1}) = \{q\}$, $N(u_{h-2}) \cap N(u_{h-1}) = \{r\}$ and $N(v_{h-2}) \cap N(v_{h-1}) = \{w\}$.

Note that $B_{\vartheta_{h-1}\vartheta_h} - q - v' - u' - u_{h-1} - v_{h-1} \cong B_{\vartheta_{h-1}\vartheta_h} - q - v' - u' - u_{h-1} - r \cong P_4$. By Lemma 2.1, we can verify that

$$\begin{aligned}\mathbf{A}(x)\mathbf{A}(x)\mathbf{e}_7 =& (2x^4(x+1), 3x^4, 2x^4, x^3(x+1), x^4, x^3(x+1), x^3, 2x^3, x^3)^\top \\ =& x^3 Z_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h} - q - v' - u' - u_{h-1} - v_{h-1}) \\ &+ x^3 Z_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h} - q - v' - u' - u_{h-1} - r).\end{aligned}$$

Then, by Lemma 2.2, we can get

$$\begin{aligned}& x^3 Z(B_{\vartheta_1\cdots\vartheta_h} - q - N[u] - v' - u' - u_{h-1} - v_{h-1}) \\ &\qquad + x^3 Z(B_{\vartheta_1\cdots\vartheta_h} - q - N[u] - v' - u' - u_{h-1} - r) \\ =& x^3 \mathbf{e}_7^\top \Big(\prod_{i=1}^{h-2} \mathbf{M}_i(x) \Big) Z_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h} - q - v' - u' - u_{h-1} - v_{h-1}) \\ &+ x^3 \mathbf{e}_7^\top \Big(\prod_{i=1}^{h-2} \mathbf{M}_i(x) \Big) Z_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h} - q - v' - u' - u_{h-1} - r) \\ =& \mathbf{e}_7^\top \Big(\prod_{i=1}^{h-2} \mathbf{M}_i(x) \Big) \mathbf{A}(x)\mathbf{A}(x)\mathbf{e}_7 = \mathbf{e}_7^\top \Big(\prod_{i=1}^{h} \mathbf{M}_i(x) \Big) \mathbf{e}_7.\end{aligned}$$

We also note that $\mathbf{A}(x)\mathbf{A}(x)\mathbf{e}_3 = (3x^4, 2x^3, x^4, x^3, 2x^3, x^3, x^3, x^2, x^2)^\top = x^2 Z_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h} - q - v' - p - u_{h-1})$. Then, by Lemma 2.2, we can get

$$\begin{aligned}& x^2 Z(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - q - v - v' - p - u_{h-1}) \\ &\quad = x^2 \mathbf{e}_3^\top \Big(\prod_{i=1}^{h-2} \mathbf{M}_i(x) \Big) Z_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h} - q - v' - p - u_{h-1}) \\ &\quad = \mathbf{e}_3^\top \Big(\prod_{i=1}^{h-2} \mathbf{M}_i(x) \Big) \mathbf{A}(x)\mathbf{A}(x)\mathbf{e}_3 = \mathbf{e}_3^\top \Big(\prod_{i=1}^{h-2} \mathbf{M}_i(x) \Big) \mathbf{e}_3.\end{aligned}$$

Let $f_1(x) = x^2 Z(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - N[u'] - N[v'] - u - v)$. Then, by Definition 2.1 and Lemma 2.2, we have

$$\begin{aligned} f_1(x) =& x^2 \mathbf{e}_4^\top Z_{uv}(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - N[u'] - N[v']) \\ =& x^2 \mathbf{e}_4^\top \Big(\prod_{i=1}^{h-2} \mathbf{M}_i(x) \Big) Z_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h} - N[u'] - N[v']). \end{aligned}$$

Thus, by applying Lemma 2.1 and the equations derived above, we have

$$\begin{aligned} xZ(F_{\vartheta_1\vartheta_2\cdots\vartheta_h} - q - v_0) =& x^2 Z(F_{\vartheta_1\vartheta_2\cdots\vartheta_h} - q - v_0 - p - u_0) \\ &+ x^2 Z(F_{\vartheta_1\vartheta_2\cdots\vartheta_h} - q - v_0 - p - u_{h-1}) \\ &+ x^3 Z(F_{\vartheta_1\vartheta_2\cdots\vartheta_h} - q - v_0 - u_0 - u_{h-1} - s - v_{h-1}) \\ &+ x^3 Z(F_{\vartheta_1\vartheta_2\cdots\vartheta_h} - q - v_0 - u_0 - u_{h-1} - s - r) \\ =& x^2 Z(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - N[u'] - N[v'] - u - v) \\ &+ x^2 Z(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - q - v - v' - p - u_{h-1}) \\ &+ x^3 Z(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - q - N[u] - v' - u' - u_{h-1} - v_{h-1}) \\ &+ x^3 Z(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - q - N[u] - v' - u' - u_{h-1} - r), \\ =& f_1(x) + \mathbf{e}_3^\top \mathbf{A}(x)\mathbf{A}(x)\mathbf{e}_3 + \mathbf{e}_7^\top \Big(\prod_{i=1}^{h-2} \mathbf{M}_i(x) \Big) \mathbf{e}_7. \end{aligned}$$

We can obtain that $x^2 Z_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h} - v_{h-1} - p - u_{h-1} - N[v']) = (x^4 + x^3, x^3, x^3, x^2, x^3, x^3, x^2, x^2, x^2)^\top = \mathbf{A}(x)\mathbf{A}(x)\mathbf{e}_1$ by the use of Lemma 2.1. Then, by Definition 2.1 and Lemma 2.2 we get

$$\begin{aligned} x^2 Z(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - v_{h-1} - p - u_{h-1} - N[v']) =& \mathbf{e}_1^\top \Big(\prod_{i=1}^{h-2} \mathbf{M}_i(x) \Big) \mathbf{A}(x)\mathbf{A}(x)\mathbf{e}_1 \\ =& \mathbf{e}_1^\top \Big(\prod_{i=1}^{h} \mathbf{M}_i(x) \Big) \mathbf{e}_1. \end{aligned}$$

Similarly, note that $\mathbf{A}(x)\mathbf{A}(x)\mathbf{e}_2 = (3x^4, x^4, 2x^3, x^3, x^3, 2x^3, x^2, x^3, x^2)^\top = x^2 Z_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h} - q - v_{h-1} - p - u')$. Then, we have

$$x^2 Z(B_{\vartheta_1\vartheta_2\cdots\vartheta_h} - q - v_{h-1} - p - u - u')$$

$$
\begin{aligned}
&=x^2\mathbf{e}_2^\top\Big(\prod_{i=1}^{h-2}\mathbf{M}_i(x)\Big)Z_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h}-q-v_{h-1}-p-u')\\
&=\mathbf{e}_2^\top\Big(\prod_{i=1}^{h-2}\mathbf{M}_i(x)\Big)\mathbf{A}(x)\mathbf{A}(x)\mathbf{e}_2=\mathbf{e}_2^\top\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_2.
\end{aligned}
$$

In light of Lemma 2.1, we obtain that $x^3Z_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h}-v_{h-1}-u_{h-1}-r-N[v'])=(2x^4,x^4,x^3,x^3,0,x^3,0,x^3,0)^\top=\mathbf{A}(x)\mathbf{A}(x)\mathbf{e}_5$. By Lemma 2.2, we get

$$
\begin{aligned}
&x^3Z(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-v_{h-1}-u-u_{h-1}-r-s-N[v'])\\
&\quad=x^3\mathbf{e}_5^\top\Big(\prod_{i=1}^{h-2}\mathbf{M}_i(x)\Big)Z_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h}-v_{h-1}-u_{h-1}-r-N[v'])\\
&\quad=\mathbf{e}_5^\top\Big(\prod_{i=1}^{h-2}\mathbf{M}_i(x)\Big)\mathbf{A}(x)\mathbf{A}(x)\mathbf{e}_5=\mathbf{e}_5^\top\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_5.
\end{aligned}
$$

Let $f_2(x)=x^3Z(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-v_{h-1}-u_{h-1}-r-N[v']-u-v)$. By Lemma 2.2, we have

$$
\begin{aligned}
f_2(x)=&x^3\mathbf{e}_4^\top Z_{uv}(B_{\vartheta_1\cdots\vartheta_h}-v_{h-1}-u_{h-1}-r-N[v'])\\
=&x^3\mathbf{e}_4^\top\Big(\prod_{i=1}^{h-2}\mathbf{M}_i(x)\Big)Z_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h}-v_{h-1}-u_{h-1}-r-N[v']).
\end{aligned}
$$

Thus, by Lemma 2.1, we can further get

$$
\begin{aligned}
xZ(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}-q-v_{h-1})=&\,x^2Z(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-q-v_{h-1}-p-u-u')\\
&+x^2Z(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-v_{h-1}-p-u_{h-1}-N[v'])\\
&+x^3Z(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-v_{h-1}-u-u_{h-1}-r-s-N[v'])\\
&+x^3Z(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-v_{h-1}-u_{h-1}-r-N[v']-u-v)\\
=&\,\mathbf{e}_2^\top\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_2+\mathbf{e}_1^\top\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_1\\
&+\mathbf{e}_5^\top\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_5+f_2(x).
\end{aligned}
$$

Similarly, we can verify that

$$x^3Z(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-v-v'-v_{h-1}-w-t-p-u_{h-1})=\mathbf{e}_6^\top\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_6,$$

$$\begin{aligned}x^3Z(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}&-N[v]-v_{h-1}-w-N[u'])\\&+x^3Z(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-N[v]-v'-v_{h-1}-u_{h-1}-p-u')\\&=\mathbf{e}_8^\top\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_8,\end{aligned}$$

and

$$\begin{aligned}&x^4Z(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-N[v]-v'-v_{h-1}-w-N[u]-u'-u_{h-1}-r)\\&\quad+x^3Z(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-N[v]-v'-v_{h-1}-u_{h-1}-p-N[u]-u')\\&\quad=\mathbf{e}_9^\top\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_9.\end{aligned}$$

So, by Lemma 2.1 and the three equations above, we have

$$\begin{aligned}&x^2(Z(F_{\vartheta_1\cdots\vartheta_h}-v_0-v_{h-1}-w-t)+Z(F_{\vartheta_1\cdots\vartheta_h}-v_0-v_{h-1}-u_{h-1}-t))\\&\quad=x^3Z(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-v-v'-v_{h-1}-w-t-p-u_{h-1})\\&\qquad+x^3Z(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-N[v]-v_{h-1}-w-N[u'])\\&\qquad+x^4Z(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-N[v]-v'-v_{h-1}-w-N[u]-u'-u_{h-1}-r)\\&\qquad+x^3Z(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-N[v]-v'-v_{h-1}-u_{h-1}-p-u')\\&\qquad+x^3Z(B_{\vartheta_1\vartheta_2\cdots\vartheta_h}-N[v]-v'-v_{h-1}-u_{h-1}-p-N[u]-u')\\&\quad=\mathbf{e}_6^\top\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_6+\mathbf{e}_8^\top\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_8+\mathbf{e}_9^\top\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_9.\end{aligned}$$

On the other hand, we can verify that

$$x^2Z(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}-v_0-v_{h-1}-w-u_0)$$

$$=x^2\mathbf{e}_4^\top\Big(\prod_{i=1}^{h-2}\mathbf{M}_i(x)\Big)Z_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h}-v'-v_{h-1}-w-u'),$$

$$x^2Z(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}-v_0-v_{h-1}-u_{h-1}-u_0)$$
$$=x^2\mathbf{e}_4^\top\Big(\prod_{i=1}^{h-2}\mathbf{M}_i(x)\Big)Z_{u_{h-2}v_{h-2}}(B_{\vartheta_{h-1}\vartheta_h}-v'-v_{h-1}-u_{h-1}-u').$$

Moreover, we can get that

$$f_1(x)+f_2(x)+x^2Z(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}-v_0-v_{h-1}-w-u_0)$$
$$+x^2Z(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}-v_0-v_{h-1}-u_{h-1}-u_0)=\mathbf{e}_4^\top\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_4.$$

Therefore, by Lemma 2.1 and the above discussion, we conclude that

$$\begin{aligned}Z(F_{\vartheta_1\vartheta_2\cdots\vartheta_h},x)=&xZ(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}-q-v_0)+xZ(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}-q-v_{h-1})\\&+x^2Z(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}-v_0-v_{h-1}-w-t)\\&+x^2Z(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}-v_0-v_{h-1}-w-u_0)\\&+x^2Z(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}-v_0-v_{h-1}-u_{h-1}-t)\\&+x^2Z(F_{\vartheta_1\vartheta_2\cdots\vartheta_h}-v_0-v_{h-1}-u_{h-1}-u_0)\\=&\mathbf{e}_1^\top\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_1+\mathbf{e}_2^\top\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_2+\mathbf{e}_3^\top\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_3\\&+\mathbf{e}_4^\top\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_4+\mathbf{e}_5^\top\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_5\\&+\mathbf{e}_6^\top\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_6+\mathbf{e}_7^\top\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_7\\&+\mathbf{e}_8^\top\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_8+\mathbf{e}_9^\top\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big)\mathbf{e}_9\\=&\mathsf{tr}\Big(\prod_{i=1}^{h}\mathbf{M}_i(x)\Big).\end{aligned}$$

Case 2: $\vartheta_{h-1}=\alpha$ and $\vartheta_h=\beta$.

Similar to Case 1, by using Lemmas 2.1 and 2.2, we can derive the

following equation.

$$Z(F_{\vartheta_1\vartheta_2\cdots\vartheta_h},x)=\begin{cases}\mathsf{tr}\Big((\prod\limits_{i=1}^{h-3}\mathbf{M}_i(x))\mathbf{A}(x)\mathbf{A}(x)\mathbf{B}(x)\Big) & \text{if } \vartheta_{h-3}=\alpha,\\ \mathsf{tr}\Big((\prod\limits_{i=1}^{h-3}\mathbf{M}_i(x))\mathbf{B}(x)\mathbf{A}(x)\mathbf{B}(x)\Big) & \text{if } \vartheta_{h-3}=\beta,\\ \mathsf{tr}\Big((\prod\limits_{i=1}^{h-3}\mathbf{M}_i(x))\mathbf{C}(x)\mathbf{A}(x)\mathbf{B}(x)\Big) & \text{if } \vartheta_{h-3}=\gamma.\end{cases}$$

Case 3: $\vartheta_{h-1}=\beta$ and $\vartheta_h=\alpha$.

Adopting a similar method as Case 1, we can get the following equation.

$$Z(F_{\vartheta_1\vartheta_2\cdots\vartheta_h},x)=\begin{cases}\mathsf{tr}\Big((\prod\limits_{i=1}^{h-3}\mathbf{M}_i(x))\mathbf{A}(x)\mathbf{B}(x)\mathbf{A}(x)\Big) & \text{if } \vartheta_{h-3}=\alpha,\\ \mathsf{tr}\Big((\prod\limits_{i=1}^{h-3}\mathbf{M}_i(x))\mathbf{B}(x)\mathbf{B}(x)\mathbf{A}(x)\Big) & \text{if } \vartheta_{h-3}=\beta,\\ \mathsf{tr}\Big((\prod\limits_{i=1}^{h-3}\mathbf{M}_i(x))\mathbf{C}(x)\mathbf{B}(x)\mathbf{A}(x)\Big) & \text{if } \vartheta_{h-3}=\gamma.\end{cases}$$

Case 4: $\vartheta_{h-1}=\vartheta_h=\beta$.

By using Lemmas 2.1 and 2.2, we can obtain

$$Z(F_{\vartheta_1\vartheta_2\cdots\vartheta_h},x)=\begin{cases}\mathsf{tr}\Big((\prod\limits_{i=1}^{h-3}\mathbf{M}_i(x))\mathbf{A}(x)\mathbf{B}(x)\mathbf{B}(x)\Big) & \text{if } \vartheta_{h-3}=\alpha,\\ \mathsf{tr}\Big((\prod\limits_{i=1}^{h-3}\mathbf{M}_i(x))\mathbf{B}(x)\mathbf{B}(x)\mathbf{B}(x)\Big) & \text{if } \vartheta_{h-3}=\beta,\\ \mathsf{tr}\Big((\prod\limits_{i=1}^{h-3}\mathbf{M}_i(x))\mathbf{C}(x)\mathbf{B}(x)\mathbf{B}(x)\Big) & \text{if } \vartheta_{h-3}=\gamma.\end{cases}$$

Case 5: $\vartheta_{h-1}=\beta$ and $\vartheta_h=\gamma$.

Similarly, we can get

$$Z(F_{\vartheta_1\vartheta_2\cdots\vartheta_h},x)=\begin{cases}\mathsf{tr}\Big((\prod\limits_{i=1}^{h-3}\mathbf{M}_i(x))\mathbf{A}(x)\mathbf{B}(x)\mathbf{C}(x)\Big) & \text{if } \vartheta_{h-3}=\alpha,\\ \mathsf{tr}\Big((\prod\limits_{i=1}^{h-3}\mathbf{M}_i(x))\mathbf{B}(x)\mathbf{B}(x)\mathbf{C}(x)\Big) & \text{if } \vartheta_{h-3}=\beta,\\ \mathsf{tr}\Big((\prod\limits_{i=1}^{h-3}\mathbf{M}_i(x))\mathbf{C}(x)\mathbf{B}(x)\mathbf{C}(x)\Big) & \text{if } \vartheta_{h-3}=\gamma.\end{cases}$$

Hence, the proof is complete. ■

Example 2.1. For the hexacyclic system depicted in Figure 1, one can get that $Z(F_{\alpha\beta\alpha\beta\alpha\beta\alpha\beta\beta\gamma\beta\beta}, x) = \mathsf{tr}\big(\big(\mathbf{A}(x)\mathbf{B}(x)\big)^4\mathbf{B}(x)\mathbf{C}(x)\mathbf{B}(x)^2\big) = 229x^{24} + 17388x^{23} + 320268x^{22} + 1883314x^{21} + 4018951x^{20} + 3283883x^{19} + 1008471x^{18} + 103372x^{17} + 2753x^{16} + 8x^{15}$ by applying Theorem 2.1. Therefore, we have fully characterized the number of maximal matchings across all possible sizes for the hexacyclic system.

Example 2.2. Oz, Cruz and Rada determined the Hosoya indices of all hollow hexagons composed of 12 hexagons [13] (see Figure 9 therein). Herein, we calculate the maximal matching polynomials of these hollow hexagons via Theorem 2.1.

- $Z(F_{\alpha\alpha\alpha\beta\beta\beta\alpha\alpha\alpha\beta\beta\beta}, x) = \mathsf{tr}\big((\mathbf{A}(x)^3\mathbf{B}(x)^3)^2\big) = 104x^{24} + 10664x^{23} + 249305x^{22} + 1748832x^{21} + 4337889x^{20} + 4066698x^{19} + 1500506x^{18} + 225908x^{17} + 14591x^{16} + 388x^{15} + 4x^{14}$;

- $Z(F_{\alpha\alpha\beta\beta\alpha\alpha\beta\beta\alpha\alpha\beta\beta}, x) = \mathsf{tr}\big((\mathbf{A}(x)^2\mathbf{B}(x)^2)^3\big) = 112x^{24} + 11352x^{23} + 256356x^{22} + 1760308x^{21} + 4259502x^{20} + 3987102x^{19} + 1505430x^{18} + 229206x^{17} + 13977x^{16} + 288x^{15}$;

- $Z(F_{\alpha\beta\alpha\alpha\beta\beta\alpha\beta\alpha\alpha\beta\beta}, x) = \mathsf{tr}\big((\mathbf{A}(x)\mathbf{B}(x)\mathbf{A}(x)^2\mathbf{B}(x)^2)^2\big) = 148x^{24} + 12992x^{23} + 268452x^{22} + 1746492x^{21} + 4137394x^{20} + 3800778x^{19} + 1400631x^{18} + 201654x^{17} + 10720x^{16} + 168x^{15} + x^{14}$;

- $Z(F_{\alpha\beta\alpha\beta\alpha\beta\alpha\beta\alpha\beta}, x) = \mathsf{tr}\big((\mathbf{A}(x)\mathbf{B}(x))^4\big) = 200x^{24} + 15528x^{23} + 290352x^{22} + 1745402x^{21} + 3908457x^{20} + 3501474x^{19} + 1235045x^{18} + 148218x^{17} + 4740x^{16} + 16x^{15}$.

The following conclusion gives a computational formula for the number of maximal matchings in a hexacyclic system.

Theorem 2.2. *The number of maximal matchings of hexacyclic system* $F_{\vartheta_1\vartheta_2\ldots\vartheta_h}$ *is*

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

where $\mathbf{M}_i = \mathbf{A}(1)$ *if* $\vartheta_i = \alpha$, $\mathbf{M}_i = \mathbf{B}(1)$ *if* $\vartheta_i = \beta$, $\mathbf{M}_i = \mathbf{C}(1)$ *if* $\vartheta_i = \gamma$.

Proof. Since $\zeta(G) = Z(G,1)$ for any graph G, the number of maximal matchings in a hexacyclic system can be directly obtained by substituting $x = 1$ into Theorem 2.1. ■

Remark. Recently, Li, Yin, and Shi [9] obtained a result on calculating the number of maximal matchings in hexacyclic systems using a method different from that presented in this paper. However, Theorem 2.1 provides an approach for characterizing the number of maximal matchings of any size.

We next show that the linear hexacyclic system is the one that attains the minimum saturation number among all hexacyclic systems of the same length.

Theorem 2.3. *Let $F_{\vartheta_1\vartheta_2\ldots\vartheta_h}$ be a hexacyclic system with h hexagons. Then $s(F_{\vartheta_1\vartheta_2\ldots\vartheta_h}) \geq h$, with equality if and only if $F_{\vartheta_1\vartheta_2\ldots\vartheta_h} \cong F_{\alpha\alpha\ldots\alpha}$.*

Proof. For an arbitrary hexacyclic system $F_{\vartheta_1\vartheta_2\ldots\vartheta_h}$ with $4h$ vertices, it admits a perfect matching, and its matching number satisfies $\mu(F_{\vartheta_1\vartheta_2\ldots\vartheta_h}) = \frac{|V(F_{\vartheta_1\vartheta_2\ldots\vartheta_h})|}{2} = 2h$. Hence, $s(F_{\vartheta_1\vartheta_2\ldots\vartheta_h}) \geq \frac{\mu(F_{\vartheta_1\vartheta_2\ldots\vartheta_h})}{2} = h$. Note that the common edges u_iv_i $(0 \leq i \leq h-1)$ shared by two adjacent hexagons of the linear hexacyclic system $F_{\alpha\alpha\ldots\alpha}$ form a maximal matching. Thus, $s(F_{\alpha\alpha\ldots\alpha}) \leq h$. Combined with the earlier inequality $s(F_{\vartheta_1\vartheta_2\ldots\vartheta_h}) \geq h$, we conclude $s(F_{\alpha\alpha\ldots\alpha}) = h$. Now, we proceed to prove the uniqueness. Suppose there exists a hexacyclic system $F^*_{\vartheta_1\vartheta_2\ldots\vartheta_h} \ncong F_{\alpha\alpha\ldots\alpha}$ with $s(F^*_{\vartheta_1\vartheta_2\ldots\vartheta_h}) = h$. Since $F^*_{\vartheta_1\vartheta_2\ldots\vartheta_h}$ has $4h$ vertices, a maximal matching M of size h saturates $2h$ of them. The remaining $2h$ unsaturated vertices must be incident to edges not in M, and there are exactly $4h$ such edges. As $F^*_{\vartheta_1\vartheta_2\ldots\vartheta_h}$ contains no vertices with degree 1, each unsaturated vertex is incident to exactly two edges not in M. Moreover, no hexagon contains three unsaturated vertices. Thus, each hexagon contains exactly two non-adjacent unsaturated vertices of degree 2. This is only possible if $F^*_{\vartheta_1\vartheta_2\ldots\vartheta_h} \cong F_{\alpha\alpha\ldots\alpha}$, contradicting the assumption. ■

3 Concluding remarks

In this paper, we derive a computational formula for the maximal matching polynomials of hexacyclic systems by means of the transfer matrix technique. We prove that the maximal matching polynomial of any hexacyclic system $F_{\vartheta_1\vartheta_2\cdots\vartheta_h}$ can be expressed as the trace of the product of h matrices, each chosen from three fixed matrices corresponding to the hexagon types α, β and γ. Consequently, the number of maximal matchings of any size in an arbitrary hexacyclic system can be directly obtained from its maximal matching polynomial. A computational formula for the total number of maximal matchings over any hexacyclic system is also established. We further show that the linear hexacyclic system uniquely achieves the minimum saturation number among all hexacyclic systems of a fixed length.

Finally, based on a thorough analysis of the maximal matching polynomials of short-length hexacyclic systems via Theorem 2.1, we propose the following conjecture for future research.

Conjecture 3.1. *Among all hexacyclic systems with $h \geq 5$ hexagons, the linear hexacyclic system $F_{\alpha\alpha\ldots\alpha}$ attains the maximum number of maximal matchings and the helical hexacyclic system $F_{\beta\beta\ldots\beta}$ attains the minimum number of maximal matchings, respectively.*

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