MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **94** (2025) 477–504
ISSN: 0340–6253
doi: 10.46793/match.94-2.477O

Laplacian Spectral Indices of Hexacyclic Systems

Almasa Odžak[a], **Lejla Smajlović**[b,*], **Lamija Šćeta**[b]

[a] *Department of Mathematics and Computer Science, University of Sarajevo, Sarajevo, 71000, Bosnia and Herzegovina*

[b] *School of Economics and Business, University of Sarajevo, Sarajevo, 71000, Bosnia and Herzegovina*

almasa.odzak@pmf.unsa.ba, lejla.smajlovic@efsa.unsa.ba, lamija.sceta@efsa.unsa.ba

(Received December 9, 2024)

Abstract

The hexacyclic system graph F_n is the graph derived from a linear hexagonal chain L_n with $n > 1$ hexagons by identifying two pairs of ends of L_n. The Möbious hexacyclic system graph M_n is the graph derived from a linear hexagonal chain L_n with $n > 1$ hexagons by identifying two pairs of ends of L_n with a twist. In this paper, we compute, in a closed form, the resolvent energy, the Laplacian and the signless Laplacian resolvent energy, as well as the resolvent Estrada index and the resolvent signless Estrada index of F_n and M_n. All five indices are expressed as a rational function in the number n of hexagons, defined in terms of Chebyshev polynomials of the first and the second kind. Those expressions allow for a fast numerical computation of indices and for deducing sharp bounds on their growth.

1 Introduction

A topological index of a graph is a graph invariant that represents a certain number associated with the graph and which further describes its struc-

*Corresponding author.

ture. The interest in studying topological indices is mainly due to their use as one of the fundamental tools in QSPR/QSAR modeling employed in different fields of chemistry in order to describe and predict physical properties and biological activities of organic compounds from their molecular structures, see e.g. [40], [59] or [24]. There exist many topological indices of graphs. Some of those are defined in terms of geometric properties of a graph, such as (minimal) distances between vertices (the Wiener index).

A topological index may also be expressed in terms of the spectrum of its adjacency matrix which then also determines the spectrum of the Laplacian or a modified Laplacian matrix associated to a graph (e.g. signless Laplacian, normalized Laplacian). The energy of a graph, introduced in [26] equals the sum of absolute values of the eigenvalues of the adjacency matrix, see also [29] and [42] for a comparative study of graph energies. The Estrada index, introduced by Estrada in [19] equals the sum $\sum_j \exp(\lambda_j)$ over all eigenvalues λ_j of the adjacency matrix of a graph. A variety of modifications of the Estrada index have been studied in the literature and defined in terms of eigenvalues of a matrix associated to the graph, such as the Laplacian, the normalized Laplacian, the signless Laplacian, and the maximum Laplacian, to name a few; see the analysis and comparison in [20] and extensive bibliography therein.

1.1 Resolvent based topological graph indices

Resolvent based indices are closely related to the spectral moments of a graph and have a vast potential in analyzing structure activity relationships. They possess high discriminating power with respect to both biological activity and physical properties of a graph model of a molecule, see e.g. [25], [50] or [21].

More precisely, for an undirected graph G on N vertices with the adjacency matrix A with eigenvalues $\lambda_1, \dots, \lambda_N$ its resolvent matrix $\mathcal{R}_A(z)$ is defined, for all complex $z \in \mathbb{C} \setminus \{\lambda_1, \dots, \lambda_N\}$ as

$$\mathcal{R}_A(z) = (zI_N - A)^{-1},$$

where I_N is the identity matrix of order N. The resolvent energy of the graph G, denoted by $ER(G)$ is defined in [34] as the sum of eigenvalues of the matrix $\mathcal{R}_A(N)$. (Note that all eigenvalues of $\mathcal{R}_A(N)$ are positive, due to the fact that $\lambda_j \leq N-1$ for all $j = 1, \ldots, N$.) The resolvent energy can be viewed as the special value at $t = N^{-1}$ of the generating function

$$\mathcal{M}_G(t) := \frac{1}{N} \sum_{k=0}^{\infty} M_k(G) t^k$$

of the spectral moments $M_k(G) = \sum_j \lambda_j^k$ of G, see [34] where certain bounds on $ER(G)$ have been deduced. Properties of the resolvent energy, for different graphs have been studied in [1], [18], [22], [71], [74].

The Laplacian resolvent energy, denoted by $RL(G)$ and associated to the Laplacian $L := D - A$, where D is the degree matrix of G, is defined in [8] as the sum of all eigenvalues of the matrix $(N+1-L)^{-1}$.

Some lower bounds for $RL(G)$ are given in [53] and sharpened in [75], [48]. The signless Laplacian resolvent energy, associated to the signless Laplacian $L^+ := D + A$, denoted by $RL^+(G)$ is defined as the sum of all eigenvalues of the matrix $(2N-1-L^+)^{-1}$.

We refer to [8] for further details and [5], [6] for properties of the normalized signless Laplacian resolvent energy.

The resolvent Estrada index associated to the graph G on N vertices, was introduced in [21] as

$$EER(G) := \sum_{k=0}^{\infty} M_k(G)(N-1)^{-k}.$$

Benzi and Boito showed in [2] that $EER(G)$ actually equals $(N-1)$ times the sum of the eigenvalues of the resolvent matrix $\mathcal{R}_A(N-1)$, in view of which the index $EER(G)$ was named. Analogously, the resolvent signless Estrada index $SLEER(G)$ is defined in [52] as $2(N-1)$ times the sum of the eigenvalues of the matrix $(2N-2-L^+)^{-1}$. Note that $EER(G)$ and $SLEER(G)$ are well defined for all graphs G different from the complete graph K_N on N vertices.

The resolvent Estrada index is further studied in [10] and [11]; the lower bounds for the index have been derived in [72], with further refinements of the bounds for both the resolvent Estrada index and the resolvent signless Laplacian Estrada index deduced in [73]. The extremal properties of the resolvent Estrada index have been studied in [33], [32], [52], and [71].

1.2 Hexagonal chains and systems

In theoretical and mathematical chemistry, hexagonal systems are one of the very important categories of structures that can be viewed as a natural graph representation of different molecules. For example, they can be considered as representations of (unbranched catacondensed) benzenoid hydrocarbons, see e.g. [28], [30], [31], [57].

There exist different types of hexagonal systems, depending on a way hexagons are connected. The simplest hexagonal system is a linear hexagonal chain with n hexagons. By identifying the end edges of a linear hexagonal chain one can create a hexacyclic or a Möbius hexacyclic chain, see Figure 1 below.

Properties of hexagonal chains have been extensively studied by mathematicians, chemists and physicists. For example, in [35] perfect matchings in random hexagonal chain graphs have been studied; the Wiener index of hexagonal chain was computed in [16], its edge-Szeged index in [61], while the Kirchhoff and the degree Kirchhoff indices of hexagonal chains were computed in [65] and [37], respectively. Global mean first passage time of random walks on a hexagonal chain was computed in [66].

The energy of directed hexagonal systems has been derived in [56], the characteristic polynomial of prolate rectangle of benzenoid system has been computed in [45], the Kirchoff index and the degree-Kirchhoff index for hexagonal Möbius graphs (chains) were obtained in [62] and [46], respectively. Pan and Li [54] computed the degree-Kirchhoff index and the number of spanning trees of the linear crossed hexagonal chains, while Huang and Li [36] determined resistance distances and Kirchhoff indices of hexagonal cylinder chains. Further recent results on properties of hexagonal chains and hexagonal systems (in chronological order) can be found in [17], [13], [4], [49], [68], [12], [64], [60], [15], [38], [69], [51], [63], [9], [67], [70], [47]; see also [16] and an extensive bibliography there.

1.3 Our main results

In spite of a very extensive bibliography related to various topological indices of hexagonal systems, the resolvent energy indices and the resolvent Estrada indices have not been evaluated for any of the hexagonal chains and systems described above.

The main purpose of this paper is to evaluate, *in a closed form* the resolvent energy, the Laplacian and the signless Laplacian resolvent energy, as well as the resolvent Estrada index and the resolvent signless Estrada index of hexacyclic system graphs F_n and Möbius hexacyclic system graphs M_n. (For more details on the structure of those graphs, see Section 2.2 below.)

The closed form evaluations of the five resolvent indices listed above are derived in corollaries 1 – 5 below. They follow from our main theorem:

Theorem 1. *Let* a, b, c, $\beta \in \mathbb{R}$ *and* $c \neq 0$ *be arbitrary constants such that* $S = \left\{ s_j^{\pm} = a \pm \sqrt{b + c\cos\left(\frac{2\pi(j+\beta)}{n}\right)} : j = 1, \ldots, n \right\}$ *is a set of* $2n \geq 2$ *non-zero numbers. Then*

$$S_n(a,b,c,\beta) := \sum_{j=1}^{n} \left(\frac{1}{s_j^+} + \frac{1}{s_j^-} \right) = \frac{2a}{c} \frac{nU_{n-1}\left(\frac{a^2-b}{c}\right)}{T_n\left(\frac{a^2-b}{c}\right) - \cos 2\pi\beta}. \tag{1}$$

Here, T_m and U_m, $m \in \mathbb{N} \cup \{0\}$ denote the Chebyshev polynomials of the first and the second kind, respectively. Those are the unique polynomials satisfying

$$T_m(\cos\theta) = \cos(m\theta),$$

$$U_m(\cos\theta)\sin\theta = \sin((m+1)\theta),$$

see [58] for their properties and a long list of applications.

Though Chebyshev polynomials have a vast number of applications, to the best of our knowledge, there is only one paper relating topological indices of graphs to Chebyshev polynomials. Namely, in [23] it is proved that the Chebyshev polynomials provide approximations to Estrada index of certain graphs.

As an illustration of our main result, we present the following corollary in which the resolvent energy of graphs F_n and M_n is expressed in terms of Chebyshev polynomials depending singly on the number n of hexagons.

Corollary 1. *The resolvent energy of the hexacyclic system graph F_n and the Möbius hexacyclic system graph M_n are*

$$\begin{aligned} ER(F_n) = \left(4n - \frac{1}{2}\right) \frac{nU_{n-1}(8n^2-2n-1)}{T_n(8n^2-2n-1)-1} \\ + \left(4n + \frac{1}{2}\right) \frac{nU_{n-1}(8n^2+2n-1)}{T_n(8n^2+2n-1)-1} \end{aligned} \tag{2}$$

and

$$\begin{aligned} ER(M_n) = \left(4n - \frac{1}{2}\right) \frac{nU_{n-1}(8n^2-2n-1)}{T_n(8n^2-2n-1)-1} \\ + \left(4n + \frac{1}{2}\right) \frac{nU_{n-1}(8n^2+2n-1)}{T_n(8n^2+2n-1)+1}. \end{aligned} \tag{3}$$

We find the new closed formulas very useful for numerical calculations since many computational tools provide very efficient and precise built-in algorithms for numerical evaluations of Chebyshev polynomials. Some calculations are presented in tables 1–4. We also notice that there is a very small difference between the resolvent energies $ER(F_n)$ and $ER(M_n)$, even for a modest value of n. This is expected because those graphs differ only in one edge twist.

Finally, the ratio of Chebyshev polynomials of large index and argument satisfy very sharp bounds, as derived in Lemma 1 below. Those bounds imply very sharp bounds for all five resolvent indices computed in this paper. For example, we show that there exists a positive constant c such that

$$\begin{aligned} EER(F_n) = (4n^2-n)\left(\frac{4n-\frac{3}{2}}{\sqrt{(8n^2-6n)^2-1}} + \frac{4n-\frac{1}{2}}{\sqrt{(8n^2-2n-1)^2-1}}\right) \\ + O(n^{-cn}), \end{aligned}$$

$$EER(F_n) = (4n^2 - n)\left(\frac{4n - \frac{3}{2}}{\sqrt{(8n^2-6n)^2-1}} + \frac{4n - \frac{1}{2}}{\sqrt{(8n^2-2n-1)^2-1}}\right) + O(n^{-cn}),$$

as $n \to \infty$.

1.4 Organization of the paper

After introducing the necessary background material and proving a bound for the ratio of Chebyshev polynomials in Section 2, we prove our main theorem in Section 3. A closed evaluation of resolvent indices is given in Section 4. Numerical computations of indices are presented in Section 5, while the asymptotic behavior of the resolvent energy and the resolvent Estrada index is derived in Section 6.

2 Preliminaries

In this section, we provide necessary background material for the paper. More precisely, we introduce resolvent based indices of a graph, define the hexacyclic system and the Möbius hexacyclic system graphs and review existing results on the spectrum of those graphs. In the last subsection, we prove a sharp inequality for a certain ratio of the Chebyshev polynomials that will be used to deduce sharp upper and lower bounds for the resolvent based indices.

2.1 Resolvent based graph indices

Let $G = (V(G), E(G))$ be a simple, undirected and unweighted graph with the set of vertices $V(G)$ having N elements and the set of edges $E(G)$. We denote by $A = A(G)$ the adjacency matrix of G and by $D = D(G)$ its degree matrix. The Laplacian matrix attached to G is defined by $L = L(G) = D(G) - A(G)$, while the signless Laplacian matrix is $L^+ = L^+(G) = D(G) + A(G)$.

The adjacency matrix is symmetric, hence its spectrum is real. Let us denote the spectrum of $A(G)$ by $\lambda_1 \le \lambda_2 \le \lambda_3 \le \ldots \le \lambda_N$, the spectrum of the Laplacian L by $\mu_1 \leq \mu_2 \leq \mu_3 \leq \ldots \leq \mu_N$, and the signless Laplacian spectrum by $q_1 \leq q_2 \leq q_3 \leq \ldots \leq q_N$. It is well known that $\lambda_N \leq N-1$, $\mu_N \leq N$ and $q_N \leq 2(N-1)$, and the equality holds true if and only if G is a complete graph K_N on N vertices, see [14].

The resolvent indices associated to A, L and L^+ are defined as follows. *The resolvent energy* of a graph G is defined in [34] by

$$ER(G) = \sum_{j=1}^{N} \frac{1}{N-\lambda_j}, \tag{4}$$

while the *Laplacian resolvent energy* and *signless Laplacian resolvent energy* are defined in [8] by

$$RL(G) = \sum_{j=1}^{N} \frac{1}{N+1-\mu_j} \tag{5}$$

and

$$RL^+(G) = \sum_{j=1}^{N} \frac{1}{2N-1-q_j}, \tag{6}$$

respectively. *The resolvent Estrada index* is defined in [21] by

$$EER(G) = \sum_{j=1}^{N} \frac{N-1}{N-1-\lambda_j} = \sum_{j=1}^{N} \left(1 - \frac{\lambda_j}{N-1}\right)^{-1}, \tag{7}$$

while the *resolvent signless Estrada index* is defined in [52] as

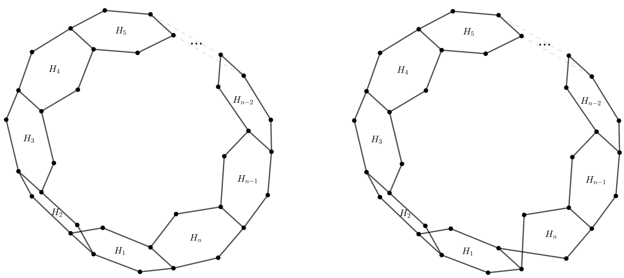
$$SLEER(G) = \sum_{j=1}^{N} \frac{2N-2}{2N-2-q_j} = \sum_{j=1}^{N} \left(1 - \frac{q_j}{2(N-1)}\right)^{-1}. \tag{8}$$

Note that the indices (4)–(6) are well-defined for all graphs, while indices (7) and (8) are well defined for all graphs different from K_N.

2.2 Linear hexacyclic system graphs and their spectra

A hexagonal system graph is a structure composed of connected hexagonal units. Different arrangements and ways of connecting these units produce various hexagonal systems. A linear hexagonal chain is a structure where hexagons are arranged in a straight sequential line with each hexagon sharing an edge with the next one. This arrangement produces a chain-like structure with unconnected ends.

The hexacyclic system F_n is a graph consisting of $n > 1$ hexagons arranged in a circular sequence, connected end-to-end to form a symmetric ring of hexagons, see Figure 1(a). The Möbius hexacyclic system a graph consisting of $n > 1$ hexagons arranged in a circular sequence, formed by twisting a hexacyclic chain before connecting its ends, introducing a single twist. It can be understood as a graph on the Möbius strip, see Figure 1(b). Graphs F_n and M_n possess $N = 4n$ vertices and $5n$ edges.



(a) Hexacyclic system F_n **(b)** Möbius hexacyclic system M_n

Figure 1. Hexagonal systems

The spectra of the adjacency matrix and of the Laplacian and signless Laplacian of graphs F_n and M_n is given in the following propositions.

Proposition 2 ([27], p. 309, [43], Corollary 4.1., see also [55], [41]).

(i) The spectrum Sp_{AF} of the adjacency matrix for the graph F_n, equals

$Sp_{AF1} \cup Sp_{AF2}$, *where*

$$Sp_{AF1} = \left\{ \frac{1}{2} \pm \sqrt{\frac{9}{4} + 2\cos\left(\frac{2\pi j}{n}\right)} : j = 1, \ldots, n \right\},$$

$$Sp_{AF2} = \left\{ -\frac{1}{2} \pm \sqrt{\frac{9}{4} + 2\cos\left(\frac{2\pi j}{n}\right)} : j = 1, \ldots, n \right\}.$$

(ii) The spectrum Sp_{AM} of the adjacency matrix for the graph M_n equals $Sp_{AM1} \cup Sp_{AM2}$, where $Sp_{AM1} = Sp_{AF1}$ and

$$Sp_{AM2} = \left\{ -\frac{1}{2} \pm \sqrt{\frac{9}{4} + 2\cos\left(\frac{(2j-1)\pi}{n}\right)} : j = 1, \ldots, n \right\}. \quad (9)$$

The spectra of the Laplacian matrices for graphs F_n and M_n are easily derived from the corresponding characteristic polynomials (see [44], Theorem 2.1 and Theorem 3.1). They are given in the following propositions.

Proposition 3 ([44], Theorems 2.2 and 3.2.)**.**

(i) The spectrum Sp_{LF} associated with the Laplacian matrix of the graph F_n equals $Sp_{LF1} \cup Sp_{LF2}$, where

$$Sp_{LF1} = \left\{ 2 \pm \sqrt{2 + 2\cos\left(\frac{2\pi j}{n}\right)} : j = 1, \ldots, n \right\},$$

$$Sp_{LF2} = \left\{ 3 \pm \sqrt{3 + 2\cos\left(\frac{2\pi j}{n}\right)} : j = 1, \ldots, n \right\}.$$

(ii) The spectrum Sp_{LM} associated with the Laplacian matrix of the graph M_n equals $Sp_{LM1} \cup Sp_{LM2}$, where $Sp_{LM1} = Sp_{LF1}$ and

$$Sp_{LM2} = \left\{ 3 \pm \sqrt{3 + 2\cos\left(\frac{(2j-1)\pi}{n}\right)} : j = 1, \ldots, n \right\}.$$

Notice that sets Sp_{LF1} and Sp_{LM1} contain the trivial eigenvalue $\mu = 0$.

The spectrum Sp_{sLF} of the signless Laplacian associated to F_n is easily deduced from the fact that F_n is a bipartite graph. Thus, from [7, Proposition 1.3.10] we see that $Sp_{sLF} = Sp_{LF}$. The signless Laplacian spectrum of M_n can be calculated using the procedure used in [44] to obtain the Laplacian spectrum. More precisely, the following proposition holds true.

Proposition 4. *(i)* $Sp_{sLF} = Sp_{LF}$.

(ii) The spectrum Sp_{sLM} *associated with the signless Laplacian matrix of the Möbius hexacyclic system graph* M_n *equals* $Sp_{sLM1} \cup Sp_{sLM2}$*, where*

$$Sp_{sLM1} = \left\{ 2 \pm \sqrt{2 + 2\cos\left(\frac{(2j-1)\pi}{n}\right)} : j = 1, \dots, n \right\},$$

$$Sp_{sLM2} = \left\{ 3 \pm \sqrt{3 + 2\cos\left(\frac{2j\pi}{n}\right)} : j = 1, \dots, n \right\}.$$

2.3 Inequalities for the Chebyshev polynomials of large order and argument

In this section we deduce two inequalities for the ratio of the Chebyshev polynomials $U_{n-1}(x)$ and $T_n(x) \pm 1$ for large levels n and arguments x. More precisely, we will prove the following lemma.

Lemma 1. *For any integer* $n \geq 1$ *and real number* $x > 1$ *we have the following inequalities*

$$\left(1 - 2e^{-2n\cosh^{-1}(x)}\right)\left(1 - 2e^{-n\cosh^{-1}(x)}\right) \leq \frac{\sqrt{x^2-1}U_{n-1}(x)}{T_n(x)+1} \leq 1 \quad (10)$$

and

$$\left(1 - 2e^{-2n\cosh^{-1}(x)}\right) \leq \frac{\sqrt{x^2-1}U_{n-1}(x)}{T_n(x)-1} \leq \left(1 + \frac{1}{\cosh(n\cosh^{-1}(x)) - 1}\right). \quad (11)$$

Here $\cosh^{-1}$ *denotes the inverse function of the function* cosh*, meaning that for all* $x > 1$ *one has* $\cosh^{-1} x = \log(x + \sqrt{x^2-1})$.

Proof. We start by observing that, for $x > 1$ we have

$$\frac{\sqrt{x^2-1}U_{n-1}(x)}{T_n(x)} = \frac{\sinh(n\cosh^{-1}(x))}{\cosh(n\cosh^{-1}(x))} = \tanh(n\cosh^{-1}(x)).$$

Trivially, for $y > 1$ one has the bounds

$$1 - 2e^{-2y} \leq \tanh y \leq 1,$$

hence

$$\frac{\sqrt{x^2-1}U_{n-1}(x)}{T_n(x)+1} \leq \frac{\sqrt{x^2-1}U_{n-1}(x)}{T_n(x)} \leq 1$$

and

$$\frac{\sqrt{x^2-1}U_{n-1}(x)}{T_n(x)-1} \geq \frac{\sqrt{x^2-1}U_{n-1}(x)}{T_n(x)} \geq 1 - 2e^{-2n\cosh^{-1}(x)}.$$

This proves the right-hand side of (10) and the left-hand side of (11). Next, we prove the left-hand side of (10)

$$\begin{aligned}
&\frac{\sqrt{x^2-1}U_{n-1}(x)}{T_n(x)+1} = \tanh(n\cosh^{-1}(x))\frac{T_n(x)}{T_n(x)+1} \\
&\geq \left(1 - 2e^{-2n\cosh^{-1}(x)}\right)\left(1 - \frac{1}{T_n(x)+1}\right) \\
&= \left(1 - 2e^{-2n\cosh^{-1}(x)}\right)\left(1 - \frac{2}{e^{n\cosh^{-1}(x)} + e^{-n\cosh^{-1}(x)} + 2}\right) \\
&\geq \left(1 - 2e^{-2n\cosh^{-1}(x)}\right)\left(1 - 2e^{-n\cosh^{-1}(x)}\right).
\end{aligned}$$

Finally, we prove the right-hand side of (11)

$$\begin{aligned}
\frac{\sqrt{x^2-1}U_{n-1}(x)}{T_n(x)-1} &= \tanh(n\cosh^{-1}(x))\left(1 + \frac{1}{T_n(x)-1}\right) \\
&\leq 1 + \frac{1}{\cosh(n\cosh^{-1}(x)) - 1}.
\end{aligned}$$

■

In a special case when $x = P_m(n)$ is a degree $m \geq 1$ polynomial in n with a positive lead coefficient, it is obvious that $\exp(-n\cosh^{-1} x)$, when $n \to \infty$ decays as n^{-cn} for some positive constant c. Therefore, from Lemma 1 we deduce that for any polynomial P_ℓ of degree $\ell \geq 1$ with a positive lead term one has that

$$\begin{aligned} P_\ell(n)\frac{U_{n-1}(P_m(n))}{T_n(P_m(n)) \pm 1} &= \frac{P_\ell(n)}{\sqrt{(P_m(n)^2 - 1)}}\left(1 + O(n^{-c_1 n})\right) \\ &= \frac{P_\ell(n)}{\sqrt{(P_m(n)^2 - 1)}} + O(n^{-c_2 n}), \end{aligned} \tag{12}$$

as $n \to \infty$, for some positive constants c_1, c_2.

3 Proof of Theorem 1

In this Section we prove Theorem 1. We start by observing that for $j = 1, 2, \ldots, n$ we have

$$\begin{aligned} \frac{1}{s_j^+} + \frac{1}{s_j^-} &= \frac{1}{a + \sqrt{b + c\cos\left(\frac{2\pi(j+\beta)}{n}\right)}} + \frac{1}{a - \sqrt{b + c\cos\left(\frac{2\pi(j+\beta)}{n}\right)}} \\ &= \frac{2a}{a^2 - b - c\cos\left(\frac{2\pi(j+\beta)}{n}\right)}. \end{aligned}$$

Therefore

$$\begin{aligned} S_n(a, b, c, \beta) &= \sum_{j=1}^{n} \frac{2a}{a^2 - b - c\cos\left(\frac{2\pi(j+\beta)}{n}\right)} \\ &= \frac{2a}{c}\sum_{j=1}^{n} \frac{1}{\frac{a^2-b-c}{c} + 2\sin^2\left(\frac{\pi(j+\beta)}{n}\right)}. \end{aligned} \tag{13}$$

It is left to evaluate the sum on the right-hand side of (13). We will apply results given in [39, relations (41) and (42)], where the following formula has been derived

$$\frac{1}{m}\sum_{j=0}^{m-1}\frac{e^{2\pi i\frac{j\ell}{m}}}{s+2\sin^2\left(\pi\frac{j+\beta}{m}\right)}=e^{2\pi i\frac{\beta\ell}{m}}\frac{U_{m-\ell-1}\left(s+1\right)+e^{2\pi i\beta}U_{\ell-1}\left(s+1\right)}{T_m\left(s+1\right)-\cos(2\pi\beta)},\tag{14}$$

for all $\ell\in\{0,1,\ldots,m-1\}$ and all complex s such that $T_m\left(s+1\right)-\cos(2\pi\beta)\neq 0$, with the convention $U_{-1}(s+1)\equiv 0$. Taking $\ell=0$ in (14), and using the fact that the terms for $j=0$ and $j=n$ are equal, gives us

$$\sum_{j=1}^{m}\frac{1}{s+2\sin^2\left(\pi\frac{j+\beta}{m}\right)}=\frac{mU_{m-1}\left(s+1\right)}{T_m\left(s+1\right)-\cos(2\pi\beta)}.\tag{15}$$

Clearly, the sum (13) is of the form (15) for $m=n$ and $s=(a^2-b-c)/c$, and it is well defined when $a^2-b-c\neq 0$ or $\beta\neq 0$. Application of the identity (15) yields (1). If $a^2-b-c=0$ and $\beta=0$, then $s_n^-=0$, which contradicts the definition of the set S, hence the sum (13) is well defined, under assumptions of the theorem. The proof is completed.

Remark. Let us note that if $c=0$, then elements in S are independent of j, thus the evaluation of the sum S_n is trivial.

Moreover, when $a^2-b-c=0$ and $\beta=0$, then $s_n^-=0$. In that case, $s_n^+=2a$ and the sum of reciprocals of non-zero elements of the set S equals

$$\frac{a}{c}\sum_{j=1}^{n-1}\frac{1}{\sin^2\left(\frac{\pi j}{n}\right)}+\frac{1}{2a},$$

for $a\neq 0$. Application of [3, Corollary 2.3.] yields that

$$\sum_{j=1}^{m-1}\frac{1}{\sin^2\left(\frac{\pi j}{m}\right)}=\frac{m^2-1}{3},$$

which implies

$$\frac{a}{c}\sum_{j=1}^{n-1}\frac{1}{\sin^2\left(\frac{\pi j}{n}\right)}+\frac{1}{2a}=\frac{a}{c}\frac{n^2-1}{3}+\frac{1}{2a}.$$

When $a^2 - b - c = 0$, $\beta = 0$ and $a = 0$ it is trivial to see that the sum of non-zero reciprocal elements of S is zero.

4 Closed form evaluation of the resolvent based indices

In this section we combine Theorem 1 with the knowledge of the spectrum of graphs F_n and M_n to deduce closed form expressions for the resolvent and the resolvent Estrada indices of those graphs in terms of n.

4.1 Resolvent energies and resolvent Estrada indices for systems F_n and M_n.

We start by proving Corrolary 1 which gives a closed formula for the resolvent energy for hexacyclic systems F_n and M_n, and then we derive closed formulas for resolvent Estrada indices for these systems.

Proof of Corollary 1. From the definition of resolvent energy (4), in view of Proposition 2 and the fact that the number of vertices of F_n is $4n$, we have

$$ER(F_n) = \sum_{j=1}^{n} \left(\frac{1}{4n - \frac{1}{2} - \sqrt{\frac{9}{4} + 2\cos\left(\frac{2\pi j}{n}\right)}} + \frac{1}{4n - \frac{1}{2} + \sqrt{\frac{9}{4} + 2\cos\left(\frac{2\pi j}{n}\right)}} \right)$$
$$+ \sum_{j=1}^{n} \left(\frac{1}{4n + \frac{1}{2} - \sqrt{\frac{9}{4} + 2\cos\left(\frac{2j\pi}{n}\right)}} + \frac{1}{4n + \frac{1}{2} + \sqrt{\frac{9}{4} + 2\cos\left(\frac{2j\pi}{n}\right)}} \right).$$

In the notation of Theorem 1, we can write the above sums as

$$ER(F_n) = S_n\left(4n - \frac{1}{2}, \frac{9}{4}, 2, 0\right) + S_n\left(4n + \frac{1}{2}, \frac{9}{4}, 2, 0\right).$$

Application of Theorem 1 completes the proof in the case of F_n. Reasoning similarly, for the graph M_n we deduce that

$$ER(M_n) = S_n\left(4n - \frac{1}{2}, \frac{9}{4}, 2, 0\right) + S_n\left(4n + \frac{1}{2}, \frac{9}{4}, 2, -\frac{1}{2}\right),$$

which, after applying Theorem 1 completes the proof of the corollary. ■

Corollary 2. *The resolvent Estrada indices for the hexacyclic system graph F_n and the Möbius system graph M_n are*

$$EER(F_n) = (4n^2 - n)\left(\left(4n - \frac{3}{2}\right)\frac{U_{n-1}(8n^2-6n)}{T_n(8n^2-6n)-1} + \left(4n - \frac{1}{2}\right)\frac{U_{n-1}(8n^2-2n-1)}{T_n(8n^2-2n-1)-1}\right)$$

and

$$EER(M_n) = (4n^2 - n)\left(\left(4n - \frac{3}{2}\right)\frac{U_{n-1}(8n^2-6n)}{T_n(8n^2-6n)-1} + \left(4n - \frac{1}{2}\right)\frac{U_{n-1}(8n^2-2n-1)}{T_n(8n^2-2n-1)+1}\right).$$

Proof. From the definition of the resolvent Estrada index (7), combined with Proposition 2, in the notation of Theorem 1 we have

$$EER(F_n) = (4n-1)\left(S_n\left(4n - \frac{3}{2}, \frac{9}{4}, 2, 0\right) + S_n\left(4n - \frac{1}{2}, \frac{9}{4}, 2, 0\right)\right).$$

Application of Theorem 1 completes the proof in the case of F_n. Similar calculations yield the result for the system M_n. Namely, in the notation of Theorem 1 we have

$$EER(M_n) = (4n-1)\left(S_n\left(4n - \frac{3}{2}, \frac{9}{4}, 2, 0\right) + S_n\left(4n - \frac{1}{2}, \frac{9}{4}, 2, -\frac{1}{2}\right)\right),$$

which, after applying Theorem 1 completes the proof. ■

4.2 Laplacian resolvent energies and the signless Estrada resolvent indices for systems F_n and M_n

By combining Theorem 1 with Propositions 3 and 4 in which the explicit evaluation of the Laplacian and the signless Laplacian spectrum for hexacyclic systems F_n and M_n is given, we derive closed formulas for the Laplacian resolvent energies and signless Estrada resolvent index. Proofs of Corollaries 3–5 are similar as above, so we omit those.

Corollary 3. *The Laplacian resolvent energy of the hexacyclic system graph F_n and the Möbius hexacyclic system graph M_n are*

$$\begin{aligned} RL(F_n) &= \left(4n^2-n\right)\frac{U_{n-1}\left(8n^2-4n-\frac{1}{2}\right)}{T_n\left(8n^2-4n-\frac{1}{2}\right)-1} \\ &\quad + \left(4n^2-2n\right)\frac{U_{n-1}\left(8n^2-8n+\frac{1}{2}\right)}{T_n\left(8n^2-4n+\frac{1}{2}\right)-1} \end{aligned}$$

and

$$\begin{aligned} RL(M_n) &= \left(4n^2-n\right)\frac{U_{n-1}\left(8n^2-4n-\frac{1}{2}\right)}{T_n\left(8n^2-4n-\frac{1}{2}\right)-1} \\ &\quad + \left(4n^2-2n\right)\frac{U_{n-1}\left(8n^2-8n+\frac{1}{2}\right)}{T_n\left(8n^2-4n+\frac{1}{2}\right)+1}. \end{aligned}$$

Corollary 4. *The signless Laplacian energy of the hexacyclic system graph F_n and the Möbius hexacyclic system graph M_n are*

$$\begin{aligned} RL^+(F_n) &= \left(8n^2-3n\right)\frac{U_{n-1}\left(32n^2-24n+\frac{7}{2}\right)}{T_n\left(32n^2-24n+\frac{7}{2}\right)-1} \\ &\quad + \left(8n^2-4n\right)\frac{U_{n-1}\left(32n^2-32n+\frac{13}{2}\right)}{T_n\left(32n^2-32n+\frac{13}{2}\right)-1} \end{aligned}$$

and

$$\begin{aligned} RL^+(M_n) &= \left(8n^2-3n\right)\frac{U_{n-1}\left(32n^2-24n+\frac{7}{2}\right)}{T_n\left(32n^2-24n+\frac{7}{2}\right)+1} \\ &\quad + \left(8n^2-4n\right)\frac{U_{n-1}\left(32n^2-32n+\frac{13}{2}\right)}{T_n\left(32n^2-32n+\frac{13}{2}\right)-1}. \end{aligned}$$

Corollary 5. *The resolvent signless Estrada index of the hexacyclic sys-*

tem graph F_n and the Möbius hexacyclic system graph M_n are

$$SLEER(F_n) = \left(8n^2 - 2n\right) \left((8n-4) \frac{U_{n-1}\left(32n^2 - 32n + 7\right)}{T_n\left(32n^2 - 32n + 7\right) - 1} \right.$$
$$\left. + (8n-5) \frac{U_{n-1}\left(32n^2 - 40n + 11\right)}{T_n\left(32n^2 - 40n + 11\right) - 1} \right)$$

and

$$SLEER(M_n) = \left(8n^2 - 2n\right) \left((8n-4) \frac{U_{n-1}\left(32n^2 - 32n + 7\right)}{T_n\left(32n^2 - 32n + 7\right) + 1} \right.$$
$$\left. + (8n-5) \frac{U_{n-1}\left(32n^2 - 40n + 11\right)}{T_n\left(32n^2 - 40n + 11\right) - 1} \right).$$

5 Numerical calculations of resolvent based indices

Based on derived formulas it is easy to calculate any of the five indices derived in corollaries 1 – 5 for systems F_n and M_n. As an example, we summarise numerical values of the resolvent energy and the resolvent Estrada index for systems F_n and M_n for different values of n in tables 1-4.

Graphs F_n and M_n are similar, hence, as n grows, the difference in corresponding values for resolvent energies and indices of F_n and M_n becomes negligible. For example, formulas for the resolvent energy of graphs F_n and M_n, (2) and (3) imply very small differences for large n. From tables 1 and 2 we can see that for $n \geq 5$ there is no difference up to 9 decimal places. Similarly, numerical calculations given in tables 3 and 4 show that for $n \geq 4$, values of the resolvent Estrada index for F_n and M_n agree up to 7 decimal places.

n	$ER(F_n)$	n	$ER(F_n)$	n	$ER(F_n)$
2	1.042429792	3	1.017886868	4	1.009929103
5	1.006316473	6	1.004372208	7	1.003205970
8	1.002451470	9	1.001935288	10	1.001566615
11	1.001294131	12	1.001087052	13	1.000925995
14	1.000798263	15	1.000695256	16	1.000610978
17	1.000541149	18	1.000482644	19	1.000433140
20	1.000390882	21	1.000354519	22	1.000323006
23	1.000295515	24	1.000271391	25	1.000250105
26	1.000231229	27	1.000214412	28	1.000199365
29	1.000185849	30	1.000173662	31	1.000162635
32	1.000152627	33	1.000143515	34	1.000135195
35	1.000127578	36	1.000120588	37	1.000114156
38	1.000108226	39	1.000102746	40	1.000097672
41	1.000092965	42	1.000088590	43	1.000084517
44	1.000080719	45	1.000077170	46	1.000073851
47	1.000070742	48	1.000067825	49	1.000065084

Table 1. Resolvent energy for hexacyclic system F_n

n	$ER(M_n)$	n	$ER(M_n)$	n	$ER(M_n)$
2	1.042032967	3	1.017886334	4	1.009929102
5	1.006316473	6	1.004372208	7	1.003205970
8	1.002451470	9	1.001935288	10	1.001566615
11	1.001294131	12	1.001087052	13	1.000925995
14	1.000798263	15	1.000695256	16	1.000610978
17	1.000541149	18	1.000482644	19	1.000433140
20	1.000390882	21	1.000354519	22	1.000323006
23	1.000295515	24	1.000271391	25	1.000250105
26	1.000231229	27	1.000214412	28	1.000199365
29	1.000185849	30	1.000173662	31	1.000162635
32	1.000152627	33	1.000143515	34	1.000135195
35	1.000127578	36	1.000120588	37	1.000114156
38	1.000108226	39	1.000102746	40	1.000097672
41	1.000092965	42	1.000088590	43	1.000084517
44	1.000080719	45	1.000077170	46	1.000073851
47	1.000070742	48	1.000067825	49	1.000065084

Table 2. Resolvent energy for Möbius hexacyclic system M_n

n	$EER(F_n)$	n	$EER(F_n)$	n	$EER(F_n)$
2	8.4556343	3	12.2569353	4	16.1811734
5	20.1401387	6	24.1143308	7	28.0965791
8	32.0836124	9	36.0737223	10	40.0659284
11	44.0596271	12	48.0544268	13	52.0500616
14	56.0463454	15	60.0431431	16	64.0403551
17	68.0379058	18	72.0357370	19	76.0338030
20	80.0320677	21	84.0305020	22	88.0290820
23	92.0277885	24	96.0266052	25	100.0255185
26	104.0245172	27	108.0235915	28	112.0227332
29	116.0219351	30	120.0211912	31	124.0204961
32	128.0198452	33	132.0192344	34	136.0186600
35	140.0181189	36	144.0176084	37	148.0171258
38	152.0166690	39	156.0162359	40	160.0158248
41	164.0154340	42	168.0150620	43	172.0147075
44	176.0143693	45	180.0140463	46	184.0137376
47	188.0134421	48	192.0131590	49	196.0128877

Table 3. Resolvent Estrada index for hexacyclic system F_n

n	$EER(M_n)$	n	$EER(M_n)$	n	$EER(M_n)$
2	8.4502924	3	12.2569247	4	16.1811734
5	20.1401387	6	24.1143308	7	28.0965791
8	32.0836124	9	36.0737223	10	40.0659284
11	44.0596271	12	48.0544268	13	52.0500616
14	56.0463454	15	60.0431431	16	64.0403551
17	68.0379058	18	72.0357370	19	76.0338030
20	80.0320677	21	84.0305020	22	88.0290821
23	92.0277885	24	96.0266052	25	100.0255185
26	104.0245172	27	108.0235915	28	112.0227332
29	116.0219351	30	120.0211912	31	124.0204961
32	128.0198452	33	132.0192344	34	136.0186600
35	140.0181189	36	144.0176084	37	148.0171258
38	152.0166690	39	156.0162359	40	160.0158248
41	164.0154340	42	168.0150620	43	172.0147075
44	176.0143693	45	180.0140463	46	184.0137376
47	188.0134421	48	192.0131590	49	196.0128877

Table 4. Resolvent Estrada index for hexacyclic system M_n

6 Asymptotic behavior of the resolvent based indices

In this section we will describe how to derive asymptotic behavior of the resolvent indices of F_n and M_n for large values of n, using sharp inequalities (10) and (11) for the Chebyshev polynomials. An asymptotic behavior of the resolvent energy and the resolvent Estrada index is given in the following corollary.

Corollary 6. *As $n \to \infty$ we have the following asymptotics*

(i) $ER(F_n) \sim 1 + O(1/n)$ and $ER(M_n) \sim 1 + O(1/n)$,

(ii) $EER(F_n) \sim 4n + O(1/n)$ and $EER(M_n) \sim 4n + O(1/n)$.

Proof. We will prove (ii). The proof of (i) is analogous (and slightly simpler, due to the absence of the linear growth in n).

We use formulas from Corrollary 1 and apply (12) twice. First, we take $P_\ell(n) = 4n - 3/2$ and $P_m(n) = 8n^2 - 6n$ to deduce

$$\left(4n - \frac{3}{2}\right) \frac{U_{n-1}(8n^2 - 6n)}{T_n(8n^2 - 6n) - 1} = \frac{4n - \frac{3}{2}}{\sqrt{(8n^2 - 6n)^2 - 1}} + O(n^{-c_1 n}),$$

as $n \to \infty$, for some constant $c_1 > 0$. Then, we take $P_\ell(n) = 4n - 1/2$ and $P_m(n) = 8n^2 - 2n - 1$ in (12) to deduce

$$\left(4n - \frac{1}{2}\right) \frac{U_{n-1}(8n^2 - 2n - 1)}{T_n(8n^2 - 2n - 1) - 1} = \frac{4n - \frac{1}{2}}{\sqrt{(8n^2 - 2n - 1)^2 - 1}} + O(n^{-c_2 n}),$$

as $n \to \infty$, for some constant $c_2 > 0$. Therefore, there exist constants c, $\tilde{c} > 0$ such that

$$EER(F_n) = (4n^2 - n) \left(\frac{4n - \frac{3}{2}}{\sqrt{(8n^2 - 6n)^2 - 1}} + \frac{4n - \frac{1}{2}}{\sqrt{(8n^2 - 2n - 1)^2 - 1}} \right) + O(n^{-cn})$$

and

$$EER(M_n) = (4n^2 - n)\left(\frac{4n - \frac{3}{2}}{\sqrt{(8n^2-6n)^2-1}} + \frac{4n - \frac{1}{2}}{\sqrt{(8n^2-2n-1)^2-1}}\right) + O(n^{-\tilde{c}n}),$$

as $n \to \infty$. Elementary calculations yield that

$$(4n^2 - n)\left(\frac{4n - \frac{3}{2}}{\sqrt{(8n^2-6n)^2-1}} + \frac{4n - \frac{1}{2}}{\sqrt{(8n^2-2n-1)^2-1}}\right) = 4n + O\left(\frac{1}{n}\right)$$

as $n \to \infty$, which completes the proof. ■

In a similar manner, by combining (12) with corollaries 3–5 it is possible to deduce asymptotic behavior of the Laplacian resolvent energies. Moreover, using inequalities (10) and (11) for the Chebyshev polynomials it is also possible to deduce sharper and more explicit asymptotics (up to $O(1/n^k)$, for any power positive integer k). We leave those questions to an interested reader.

***Acknowledgment*:** The authors are grateful to the anonymous referee for their comments, which helped to improve the exposition of the paper.

References

[1] L. E. Allem, J. Capaverde, V. Trevisan, I. Gutman, E. Zogić, E. Glogić, Resolvent energy of unicyclic, bicyclic and tricyclic graphs, *MATCH Commun. Math. Comput. Chem.* **77** (2017) 95–104.

[2] M. Benzi, P. Boito, Quadrature rule-based bounds for functions of adjacency matrices, *Lin. Algebra Appl.* **433** (2010) 637–652.

[3] B. C. Berndt, B. P. Yeap, Explicit evaluations and reciprocity theorems for finite trigonometric sums, *Adv. Appl. Math.* **29** (2002) 358–385.

[4] L. Berrocal, A. Olivieri, J. Rada, Extremal values of vertex–degree–based topological indices over hexagonal systems with fixed number of vertices, *Appl. Math. Comput.* **243** (2014) 176–183.

[5] Ş. B. Bozkurt Altındağ, M. Matejić, I. Milovanović, E. Milovanović, Some new inequalities on the normalized signless Laplacian resolvent energy of graphs, *Asian-Eur. J. Math.* **16** (2023) #2350192.

[6] Ş. B. Bozkurt Altındağ, I. Milovanović, E. Milovanović, M. Matejić, On normalized signless Laplacian resolvent energy, *Kragujevac J. Math.* **48** (2024) 673–687.

[7] A. E. Brouwer, W. H. Haemers, *Spectra of Graphs*, Springer, New York, 2011.

[8] A. Cafure, D. A. Jaume, L. N. Grippo, A. Pastin, M. D. Safe, V. Trevisan, I. Gutman, Some results for the (signless) Laplacian resolvent, *MATCH Commun. Math. Comput. Chem.* **77** (2017) 105–114.

[9] D. Chen, X. Ma, H. Bian, Degree-Kirchhoff indices and Gutman indices of spiro and polyphenyl hexagonal chains, *Polyc. Arom. Comp.* **43** (2022) 7700–7718.

[10] X. Chen, J. Qian, Bounding the resolvent Estrada index of a graph, *J. Math. Study* **45** (2012) 159–166.

[11] X. Chen, J. Qian, On resolvent Estrada index, *MATCH Commun. Math. Comput. Chem.* **73** (2015) 163–174.

[12] R. Cruz, F. Duque, J. Rada, Hexagonal systems with minimal number of inlets, *MATCH Commun. Math. Comput. Chem.* **76** (2016) 707–722.

[13] R. Cruz, H. Giraldo, J. Rada, Extremal values of vertex-degree topological indices over hexagonal systems, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 501–512.

[14] D. Cvetković, P. Rowlinson, S. K. Simić, *An Introduction to the Theory of Graph Spectra*, Cambridge Univ. Press, Cambridge, 2009.

[15] A. A. Dobrynin, Hexagonal chains with segments of equal lengths having distinct sizes and the same Wiener index, *MATCH Commun. Math. Comput. Chem.* **78** (2017) 121–132.

[16] A. A. Dobrynin, I. Gutman, S. Klavžar, P. Zigert, Wiener index of hexagonal systems, *Acta Appl. Math.* **72** (2002) 247–294.

[17] T. Došlić, A. Graovac, O. Ori, Eccentric connectivity index of hexagonal belts and chains, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 745–752.

[18] Z. Du, Asymptotic expressions for resolvent energies of paths and cycles, *MATCH Commun. Math. Comput. Chem.* **77** (2017) 85–94.

[19] E. Estrada, Characterization of 3D molecular structure, *Chem. Phys. Lett.* **319** (2000) 713–718.

[20] E. Estrada, The many facets of the Estrada indices of graphs and networks, *SeMA J.* **79** (2022) 57–125.

[21] E. Estrada, D. J. Higham, Network properties revealed through matrix functions, *SIAM Rev.* **52** (2010) 696–714.

[22] A. Farrugia, The increase in the resolvent energy of a graph due to the addition of a new edge, *Appl. Math. Comput.* **321** (2018) 25–36.

[23] Y. Ginosar, I. Gutman, T. Mansour, M. Schork, Estrada index and Chebyshev polynomials, *Chem. Phys. Lett.* **454** (2008) 145–147.

[24] H. González-Díaz, S. Arrasate, A. G. Juan, N. Sotomayor, E. Lete, A. Speck-Planche, J. M. Ruso, F. Luan, M. N. Cordeiro, Matrix trace operators: from spectral moments of molecular graphs and complex networks to perturbations in synthetic reactions, micelle nanoparticles, and drug ADME processes, *Curr. Drug Metab.* **15** (2014) 470–488.

[25] H. González-Díaz, L. Saíz-Urra, R. Molina, Y. González-Dáz, A. Sánchez-González, Computational chemistry approach to protein kinase recognition using 3D stochastic van der Waals spectral moments, *J. Comput. Chem.* **28** (2007) 1042–1048.

[26] I. Gutman, The energy of a graph, *Ber. Math. Statist. Sekt. Forschungsz. Graz* **103** (1978) 1–22.

[27] I. Gutman, Spectral properties of some graphs derived from bipartite graphs, *MATCH Commun. Math. Comput. Chem.* **8** (1980) 291–314.

[28] I. Gutman, Topological properties of benzenoid systems, *Topics Curr. Chem.* **162** (1992) 1–28.

[29] I. Gutman, Comparative studies of graph energies, *Bull. Acad. Serbe Sci. Arts (Cl. Sci. Math. Nature.)* **144** (2012) 1–17.

[30] I. Gutman, D. Babić, Characterization of all-benzenoid hydrocarbons, *J. Mol. Struct. (Theochem)* **251** (1991) 367–373.

[31] I. Gutman, S. J. Cyvin, *Introduction to the Theory of Benzenoid Hydrocarbons*, Springer Verlag, Berlin, 1989.

[32] I. Gutman, B. Furtula, X. Chen, J. Qian, Graphs with smallest resolvent Estrada indices, *MATCH Commun. Math. Comput. Chem.* **73** (2015) 267–270.

[33] I. Gutman, B. Furtula, X. Chen, J. Qian, Resolvent Estrada index – computational and mathematical studies, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 431–440.

[34] I. Gutman, B. Furtula, E. Zogić, E. Glogić, Resolvent energy of graphs, *MATCH Commun. Math. Comput. Chem.* **75** (2016) 279–290.

[35] I. Gutman, J. W. Kennedy, L. V. Quintas, Perfect mathchings in random hexagonal chain graphs, *J. Math. Chem.* **6** (1991) 377–383.

[36] S. Huang, S. Li, On the resistance distance and Kirchhoff index of a linear hexagonal (cylinder) chain, *Phys. A: Stat. Mech. Appl.* **558** (2020) #124999.

[37] J. Huang, S. Li, L. Sun, The normalized Laplacians, degree-Kirchhoff index and the spanning trees of linear hexagonal chains, *Discr. Appl. Math.* **207** (2006) 67–79.

[38] S. Huang, S. Li, M. Zhang, On the extremal Mostar indices of hexagonal chains, *MATCH Commun. Math. Comput. Chem.* **84** (2020) 249–271.

[39] J. Jorgenson, A. Karlsson, L. Smajlović, The resolvent kernel on the discrete circle and twisted cosecant sums, *J. Math. Anal. Appl.* **538** (2024) #128454.

[40] M. Karelson, V. S. Lobanov, A. R. Katritzky, Quantum-chemical descriptors in QSAR / QSPR studies, *Chem. Rev.* **96** (1996) 1027–1044.

[41] R. F. Langler, G. Salgado, C. Mendizabal, Hückel and Möbius annulenes: Relationships between their Hückel-level orbitals and their Hückel-level energies, *Quim. Nova* **23** (2000) 841–844.

[42] X. Li, Y. Shi, I. Gutman, *Graph Energy*, Springer, New York, 2012.

[43] Z. Z. Lou, Q. X. Huang, On the characteristic polynomial of a hexagonal system and its application, *J. Math. Res. Appl.* **34** (2014) 265–277.

[44] Z. Lou, Q. Huang, X. Ma, The Laplacian spectra and Laplacian energies of hexagonal cyclic chains, *Ars Comb.* **144** (2019) 281–291.

[45] Z. Lou, Q. Huang, D. Yin, On the characteristic polynomial and the spectrum of a hexagonal system, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 153–164.

[46] X. Ma, H. Bian, The normalized Laplacians, degree-Kirchhoff index and the spanning trees of hexagonal Möbius graphs, *Appl. Math. Comput.* **355** (2019) 33–46.

[47] X. Ma, Y. Yang, Enumeration of spanning trees containing perfect matchings in hexagonal chains with a unique kink, *Appl. Math. Comput.* **475** (2024) #128722..

[48] M. Matejić, E. Zogić, E. Milovanović, I. Milovanović, A note on the Laplacian resolvent energy of graphs, *Asian-Eur. J. Math.* **13** (2020) #2050119.

[49] N. Milosavljević, D. Stevanović, Detour index of hexagonal chains, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 137–152.

[50] C. R. Munteanu, J. M. Vázquez, J. Dorado, A. P. Sierra, A. Sánchez-González, F. J. Prado-Prado, H. González-Díaz, Complex network spectral moments for ATCUN motif DNA cleavage: first predictive study on proteins of human pathogen parasites, *J. Proteome Res.* **8** (2009) 5219–5228.

[51] M. F. Nadeem, M. Azeem, A. Khalil, The locating number of hexagonal Möbius ladder network, *J. Appl. Math. Comput.* **66** (2021) 149–165.

[52] R. Nasiri, H. R. Ellahi, A. Gholami, G. H. Fath-Tabar, A. R. Ashrafi, Resolvent Estrada and signless Laplacian Estrada indices of graphs, *MATCH Commun. Math. Comput. Chem.* **77** (2017) 157–176.

[53] J. L. Palacios, Lower bounds for the Laplacian resolvent energy via majorization, *MATCH Commun. Math. Comput. Chem.* **79** (2018) 367–370.

[54] Y. Pan, J. Li, Kirchhoff index, multiplicative degree-Kirchhoff index and spanning trees of the linear crossed hexagonal chains, *Int. J. Quantum Chem.* **118** (2018) #e25787.

[55] O. E. Polansky, Relations between the roots of the acyclic and the characteristic polynomials of Hückel and Möbius cycles - Eigenvalues of certain Hückel and Möbius forms of polyacenes, *MATCH Commun. Math. Chem.* **14** (1983) 47–70.

[56] J. Rada, I. Gutman, R. Cruz, The energy of directed hexagonal systems, *Lin. Algebra Appl.* **439** (2013) 1825–1833.

[57] M. Randić, Aromaticity of polycyclic conjugated hydrocarbons, *Chem. Rev.* **103** (2003) 3449–3605.

[58] T. J. Rivlin, *Chebyshev Polynomials*, Wiley, New York, 1990.

[59] T. W. Schultz, M. T. D. Cronin, J. D. Walker, A. O. Aptula, Quantitative structure-activity relationships (QSARS) in toxicology: a historical perspective, *J. Mol. Struct.* **622** (2003) 1–22.

[60] C. Song, Q. Huang, The characteristic polynomial of a kind of hexagonal system and its application, *Ars Comb.* **127** (2016) 209–223.

[61] S. Z. Wang, B. L. Liu, A method of calcutaing the edge–Szeged index of hexagonal chain, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 91–96.

[62] G. Wang, B. Xu, Kirchhoff index of hexagonal Möbius graphs, in: *2011 International Conference on Multimedia Technology*, 2011, pp. 5912–5915.

[63] Q. Xiao, M. Zeng, Z. Tang, H. Deng, H. Hua, Hexagonal chains with first three minimal Mostar indices, *MATCH Commun. Math. Comput. Chem.* **85** (2021) 47–61.

[64] S. J. Xu, H. P. Zhang, J. Z. Cai, Complete forcing numbers of catacondensed hexagonal systems, *J. Comb. Optim.* **29** (2015) 803–814.

[65] Y. Yang, H. Zhang, Kirchhoff index of linear hexagonal chains, *Int. J. Quantum Chem.* **108** (2008) 503–512.

[66] X. Yu, S. Zaman, A. Ullah, G. Saedi, X. Zhang, Matrix analysis of hexagonal model and its applications in global mean-first-passage time of random walks, *IEEE Access* **11** (2023) 10044–10052.

[67] S. Zaman, A. N. A. Koam, A. Al Khabyah, A. Ahmad, The Kemeny's constant and spanning trees of hexagonal ring network, *Comput. Mater. Contin.* **73** (2022) 6347–6365.

[68] H. P. Zhang, J. Z. Cai, On the global forcing number of hexagonal systems, *Discr. Appl. Math.* **162** (2014) 334–347.

[69] L. Zhang, Q. Li, S. Li, M. Zhang, The expected values for the Schultz index, Gutman index, multiplicative degree-Kirchhoff index and additive degree-Kirchhoff index of a random polyphenylene chain, *Discr. Appl. Math.* **282** (2020) 243–256.

[70] S. Zhao, Matching forcing polynomials of constructable hexagonal systems, *MATCH Commun. Math. Comput. Chem.* **88** (2022) 767–797.

[71] Z. Zhu, Some extremal properties of the resolvent energy, Estrada and resolvent Estrada indices of graphs, *J. Math. Anal. Appl.* **447** (2017) 957–970.

[72] Z. Zhu, Y. Hong, M. Jiang, A unified approach to lower bound on resolvent Estrada index and resolvent energy of graphs, *J. Comb. Math. Comb. Comput.* **103** (2017) 139–146.

[73] E. Zogić, B. Borovićanin, E. Glogić, I. Milovanović, E. Milovanović, New bounds for some spectrum-based topological indices of graphs, *MATCH Commun. Math. Comput. Chem.* **86** (2021) 685–701.

[74] E. Zogić, E. Glogić, New bounds for the resolvent energy of graphs, *Sci. Publ. State Univ. Novi Pazar, Ser. A: Appl. Math. Inf. Mech.* **9** (2017) 187–191.

[75] E. Zogić, E. Glogić, A note on the Laplacian resolvent energy, Kirchhoff index and their relations, *Discr. Math. Lett.* **2** (2019) 32–37.