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*Corresponding author: Saeid Alikhani,
Department of Mathematics, Yazd
University, Yazd 89195-741, Iran
E-mail: alikhani@yazd.ac.ir

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Hari M. Srivastava, University of Victoria,
Canada

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COMPUTATIONAL SCIENCE | RESEARCH ARTICLE

Hosoya polynomial of some cactus chains

Ali Sadeghieh¹, Saeid Alikhani^{2*}, Nima Ghanbari² and Abdul Jalil M. Khalaf³

Abstract: Let $G = (V, E)$ be a simple graph. Hosoya polynomial of G is $H(G, x) = \sum_{\{u,v\} \subseteq V(G)} x^{d(u,v)}$, where $d(u, v)$ denotes the distance between vertices u and v . A cactus graph is a connected graph in which no edge lies in more than one cycle. In this paper we compute the Hosoya polynomial of some cactus chains. As a consequence, Wiener and hyper-Wiener indices of these kind of chains are also obtained.

Subjects: Science; Mathematics & Statistics; Technology; Computer Science

Keywords: Hosoya polynomial; Wiener index; hyper-Wiener index; cactus chain

AMS subject classifications: 05C12

1. Introduction

A simple graph $G = (V, E)$ is a finite nonempty set $V(G)$ of objects called vertices together with a (possibly empty) set $E(G)$ of unordered pairs of distinct vertices of G called edges. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds. The Hosoya polynomial of a graph is a generating function about distance distributing, introduced by Hosoya (1988) and for a connected graph G is defined as:

$$H(G, x) = \sum_{\{u,v\} \subseteq V(G)} x^{d(u,v)},$$

where $d(u, v)$ denotes the distance between vertices u and v . This polynomial has computed for some nano-structures (e.g. Alikhani & Iranmanesh, 2014; Xu & Zhang, 2009). The Hosoya polynomial

ABOUT THE AUTHORS



Ali Sadeghieh

Ali Sadeghieh is an assistant professor of Pure Mathematics (Algebra) in the department of Mathematics, College of Science of Yazd Branch of Islamic Azad University.

Saeid Alikhani is an associate professor of Mathematics at Yazd University, Yazd, Iran. He is managing editor of journal entitled "Algebraic structures and their applications (ASTA)" and is a member of editorial board of six international journals and a reviewer of more than 20 international journals.

Nima Ghanbari is a PhD student of Pure Mathematics (Algebraic Graph Theory) at Yazd University. He is interested to some kind of graph colorings and Mathematical Chemistry.

Abdul Jalil M. Khalaf is an assistant professor of Mathematics (Graph Theory) in Faculty of Computer Science and Mathematics, at University of Kufa, Iraq. He is interested to chromatic polynomial and chromaticity of graphs, labeling of graphs and some another graph polynomials.

PUBLIC INTEREST STATEMENT

A simple graph $G = (V, E)$ is a finite nonempty set V of objects called vertices together with a (possibly empty) set E of unordered pairs of distinct vertices of G called edges. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds. A graphical invariant is a number related to a graph which is structural invariant, that is to say it is fixed under graph automorphisms. In chemistry and for chemical graphs, these invariant numbers are known as the topological indices. One of the most important topological indices is the Wiener index of a connected graph G is denoted by $W(G)$, is the sum of distances between all pairs of vertices in G . It found numerous applications. The first derivative of the Hosoya polynomial at $x = 1$ is equal to the Wiener index. In this paper we computed the Hosoya polynomial of some cactus chains that are of importance in chemistry.

has many chemical applications (Deutsch & Klavžar, 2013; Estrada, Ivanciuc, Gutman, Gutierrez, & Rodriguez, 1998; Gutman, Klavžar, Petkovsek, & Zigert, 2001; Gutman et al., 2012). Especially, the two well-known topological indices, i.e. Wiener index and hyper-Wiener index, can be directly obtained from the Hosoya polynomial. The Wiener index of a connected graph G is denoted by $W(G)$, is defined as the sum of distances between all pairs of vertices in G (Hosoya, 1971), i.e.

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v).$$

The hyper-Wiener index is denoted by $WW(G)$ and defined as follows:

$$WW(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} d(u,v) + \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} d^2(u,v).$$

Note that the first derivative of the Hosoya polynomial at $x = 1$ is equal to the Wiener index:

$$W(G) = (H(G, x))' |_{x=1}.$$

Also we have the following relation:

$$WW(G) = \frac{1}{2} (xH(G, x))'' |_{x=1}.$$

In this paper we consider a class of simple linear polymers called cactus chains. Cactus graphs were first known as Husimi tree, they appeared in the scientific literature sixty years ago in papers by Husimi and Riddell concerned with cluster integrals in the theory of condensation in statistical mechanics (Harary & Uhlenbeck, 1953; Husimi, 1950; Riddell, 1951). We refer the reader to papers (Chellali, 2006; Majstorović, Došlić, & Klobučar, 2012) for some aspects of parameters of cactus graphs. A cactus graph is a connected graph in which no edge lies in more than one cycle. Consequently, each block of a cactus graph is either an edge or a cycle. If all blocks of a cactus G are cycles of the same size i , the cactus is i -uniform. The cactus graphs whose are i -uniform for $i = 3, 4, 6$ are of importance in chemistry and so we consider them in this paper. A triangular cactus is a graph whose blocks are triangles, i.e. a 3-uniform cactus. A vertex shared by two or more triangles is called a cut-vertex. If each triangle of a triangular cactus G has at most two cut-vertices, and each cut-vertex is shared by exactly two triangles, we say that G is a chain triangular cactus. By replacing triangles in these definitions by cycles of length 4 we obtain cacti whose every block is C_4 . We call such cacti square cacti. Note that the internal squares may differ in the way they connect to their neighbors. If their cut-vertices are adjacent, we say that such a square is an ortho-square; if the cut-vertices are not adjacent, we call the square a para-square (Alikhani, Jahari, Mehryar, & Hasni, 2014).

In the next section, we compute the Hosoya polynomial of triangular and square cacti chains. In Section 3, we compute this polynomial for two kind of chain hexagonal cactus. As a consequence, the Wiener and the hyper-Wiener indices of these kind of chains are also obtained.

2. Hosoya polynomial of triangular and square cactus chains

In this section we compute the Hosoya polynomial of triangular and square cactus chains. First we consider a chain triangular. An example of a chain triangular cactus is shown in Figure 1. We call the number of triangles in G , the length of the chain. Obviously, all chain triangular cacti of the same length are isomorphic. Hence, we denote the chain triangular cactus of length n by T_n . Here we compute the Hosoya polynomial of T_n .

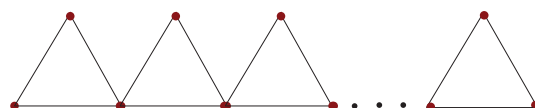


Figure 1. Chain triangular cactus T_n .

Figure 2. Para-chain square cactus graph Q_n

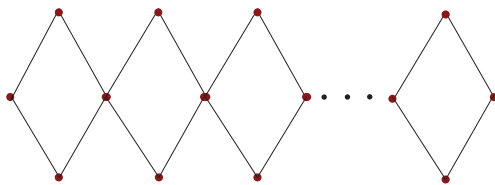
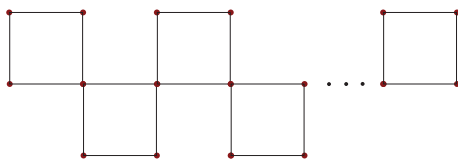


Figure 3. Ortho-chain square cactus graph O_n



THEOREM 2.1 The Hosoya polynomial of the chain triangular cactus T_n ($n \geq 2$) is

$$H(T_n, x) = 3nx + \sum_{k=2}^{n-1} (4n - 4k + 4)x^k + 4x^n.$$

Proof Let u and v be two arbitrary vertices of T_n . Suppose that $d(u, v) = k$. For $k = 1$, there are two such pair of vertices with $\deg(u) = \deg(v) = 2$, there are $2n$ pair of vertices with $\deg(u) = 2$ and $\deg(v) = 4$, and there are $n - 2$ such pair of vertices with $\deg(u) = \deg(v) = 4$. Therefore the coefficient of x in $H(T_n, x)$ is $3n$. For $2 \leq k \leq n - 1$, there are $n - k + 3$ pair of vertices u, v with $\deg(u) = \deg(v) = 2$, and $2(n - k + 1)$ pair of vertices $u, v \in V(G)$ with $\deg(u) = 2$ and $\deg(v) = 4$, and $n - k - 1$ pair of vertices such as $u, v \in V(G)$ with $\deg(u) = \deg(v) = 4$. So the coefficient of x^k for $2 \leq k \leq n - 1$ is $4n - 4k + 4$. Finally for $k = n$, there are four pair of vertices $u, v \in V(G)$ with $\deg(u) = \deg(v) = 2$, and so the coefficient of x^n is 4 . Therefore by definition of Hosoya polynomial we have the result. \square

The following corollary gives the Wiener index and hyper-Wiener index of T_n :

COROLLARY 2.2

(i) The Wiener index of triangular cactus T_n ($n \geq 2$) is

$$W(T_n) = 7n + 4 \sum_{k=2}^{n-1} k(n - k + 1).$$

(ii) The hyper-Wiener index of T_n ($n \geq 2$) is

$$WW(T_n) = n(2n + 5) + 2 \sum_{k=2}^{n-1} k(k + 1)(n - k + 1).$$

Proof

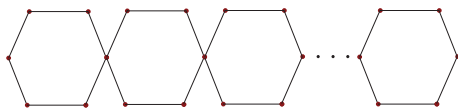
(i) It follows from Theorem 2.1 and the identity $W(G) = (H(G, x))'|_{x=1}$.

(ii) It follows from Theorem 2.1 and the identity

$$WW(G) = \frac{1}{2} (xH(G, x))''|_{x=1}.$$

By replacing triangles in the definitions of triangular cactus T_n by cycles of length 4 we obtain cacti whose every block is C_4 . We call such cacti, square cacti. An example of a square cactus chain is shown in Figure 2. We see that the internal squares may differ in the way they connect to their neighbors. If their cut-vertices are adjacent, we say that such a square is an ortho-square; if the cut-vertices are not adjacent, we call the square a para-square. We consider a para-chain of length n ,

Figure 4. Para-chain hexagonal cactus graph L_n .



which is denoted by Q_n as shown in Figure 2. The following theorem gives the Hosoya polynomial of Q_n .

THEOREM 2.3 *The Hosoya polynomial of the para-chain square cactus graph Q_n ($n \geq 2$) is*

$$H(Q_n, x) = (6n - 4)x^2 + \sum_{s=0}^{n-2} (4n - 4s)x^{2s+1} + \sum_{s=2}^{n-1} (5n - 5s + 1)x^{2s} + 4x^{2n-1} + x^{2n}.$$

Proof Suppose that u and v are two arbitrary vertices of Q_n and let $d(u, v) = k$. For $k = 2s + 1$ ($0 \leq s \leq n - 2$), there are four pair of vertices u, v with $\deg(u) = \deg(v) = 2$, there are $4(n - s - 1)$ pair of vertices u, v with $\deg(u) = 2$ and $\deg(v) = 4$. So the coefficient of x^{2s+1} is $4n - 4s$. For $k = 2$, there are $5(n - 1) + 1$ pair of vertices u, v with $\deg(u) = \deg(v) = 2$, there are two pair of vertices u, v with $\deg(u) = 2$ and $\deg(v) = 4$ and there are $n - 2$ pair of vertices such as u, v with $\deg(u) = \deg(v) = 4$. So the degree of x^2 is $6n - 4$. For $k = 2s$ ($2 \leq s \leq n - 1$), there are $4(n - s)$ pair of vertices u, v with $\deg(u) = \deg(v) = 2$, there are two pair of vertices u, v with $\deg(u) = 2$ and $\deg(v) = 4$, and there are $n - s - 1$ pair of vertices u, v with $\deg(u) = \deg(v) = 4$. So the coefficient of x^{2s} ($2 \leq s \leq n - 1$) is $5n - 5s + 1$. For $k = 2n - 1$, there are four pair of vertices u, v with $\deg(u) = \deg(v) = 2$ and for $k = 2n$, there is one pair of vertices u, v with $\deg(u) = \deg(v) = 2$. Therefore by the definition of Hosoya polynomial, we have the result. \square

The following corollary gives the Wiener index and hyper-Wiener index of Q_n Figure 5:

COROLLARY 2.4

(i) The Wiener index of the para-chain square cactus Q_n ($n \geq 2$) is

$$W(Q_n) = 22n - 12 + 4 \sum_{s=0}^{n-2} (2s + 1)(n - s) + \sum_{s=2}^{n-1} 2s(5n - 5s + 1).$$

(ii) The hyper-Wiener index of Q_n ($n \geq 2$) is

$$WW(Q_n) = 10n^2 + 15n - 12 + 4 \sum_{s=0}^{n-2} (s + 1)(2s + 1)(n - s) + \sum_{s=2}^{n-1} s(2s + 1)(5n - 5s + 1).$$

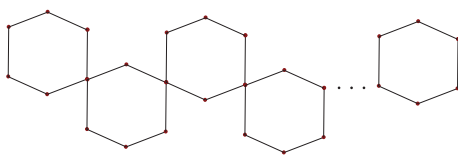
Now we consider another kind of square cactus chain and compute its Hosoya polynomial (Figure 3).

THEOREM 2.5 *The Hosoya polynomial of the ortho-chain square cactus graph O_n ($n \geq 5$) is*

$$H(O_n, x) = x^{n+2} + 6x^{n+1} + 15x^n + \sum_{k=4}^{n-1} (9n - 9k + 15)x^k + (8n - 12)x^3 + (6n - 4)x^2 + 4nx.$$

Proof Suppose that u and v are two vertices of O_n and let $d(u, v) = k$. For $k = 1$, there are $n + 2$ of vertices u, v with $\deg(u) = \deg(v) = 2$, there are $2n$ pair of vertices u, v with $\deg(u) = 2$ and $\deg(v) = 4$, and there are $n - 2$ pair of vertices such as u, v with $\deg(u) = \deg(v) = 4$. So the coefficient of x in $H(O_n, x)$ is

Figure 5. Meta-chain graph M_n .



$4n$. For $k = 2$, there are $n + 3$ pair of vertices u, v with $\deg(u) = \deg(v) = 2$, there are $4(n - 1)$ pair of vertices u, v with $\deg(u) = 2$ and $\deg(v) = 4$, and there are $n - 3$ pair of vertices u, v with $\deg(u) = \deg(v) = 4$. So the coefficient of x^2 in $H(O_n, x)$ is $6n - 4$. For $k = 3$ there are $3n$ pair of vertices u, v with $\deg(u) = \deg(v) = 2$, there are $4(n - 3) + 4$ pair of vertices u, v with $\deg(u) = 2$ and $\deg(v) = 4$, and there are $n - 4$ pair of vertices u, v with $\deg(u) = \deg(v) = 4$. So the coefficient of x^3 in $H(O_n, x)$ is $8n - 14$.

For $4 \leq k \leq n - 1$, there are $4(n - k + 3)$ pair of vertices u, v with $\deg(u) = \deg(v) = 2$, there are $4(n - k + 1)$ pair of vertices u, v with $\deg(u) = 2$ and $\deg(v) = 4$ and $n - k - 1$ pair of vertices such as u, v with $\deg(u) = \deg(v) = 4$. So the coefficient of x^k ($4 \leq k \leq n - 1$) in $H(O_n, x)$ is $(9n - 9k + 13)$. For $k = n$ there are 13 pairs of vertices u, v with $\deg(u) = \deg(v) = 2$, there are two pairs of vertices u, v with $\deg(u) = 2$ and $\deg(v) = 4$. So the coefficient of x^n in $H(O_n, x)$ is 15. Finally observe that there are six pairs of vertices u, v with $d(u, v) = n + 1$ and one pair of vertices such as u, v with $d(u, v) = n + 2$. Therefore we have the result. \square

The following corollary gives the Wiener index and the hyper-Wiener index of O_n .

COROLLARY 2.6

(i) The Wiener index of the ortho-chain square cactus graph O_n ($n \geq 5$) is

$$W(O_n) = 62n - 36 + \sum_{k=4}^{n-1} k(9n - 9k + 15).$$

(ii) The hyper-Wiener index of O_n ($n \geq 5$) is

$$WW(O_n) = 11n^2 + 55n - 51 + \frac{1}{2} \sum_{k=4}^{n-1} k(k + 1)(9n - 9k + 15).$$

3. Hosoya polynomial of chain hexagonal cactus

In this section we shall compute the Hosoya polynomial of some hexagonal cactus chains. By replacing triangles in the definitions of triangular cactus, by cycles of length 6 we obtain cacti whose every block is C_6 . We call such cacti, hexagonal cacti. An example of a hexagonal cactus chain is shown in Figure 4. We see that the internal hexagonal may differ in the way they connect to their neighbors. If their cut-vertices are adjacent, we say that such a square is an ortho-hexagonal; if the cut-vertices are not adjacent, we call the square a para-hexagonal. We consider a para-chain of length n , which is denoted by L_n as shown in Figure 4. The following theorem gives the Hosoya polynomial of L_n . In this section, we shall compute the Hosoya polynomial of two kinds of para-chain hexagonal cactus. The following theorem gives the Hosoya polynomial of L_n .

THEOREM 3.1 *The Hosoya polynomial of the para-chain hexagonal cactus graph L_n ($n \geq 3$) is*

$$H(L_n, x) = x^{3n} + 4x^{3n-1} + 8x^{3n-2} + \sum_{s=2}^{n-1} (9n - 9s + 1)x^{3s} + \sum_{s=1}^{n-2} (8n - 8s - 4)x^{3s+2} + \sum_{s=1}^{n-2} 8(n - s)x^{3s+1} + (11n - 8)x^3 + (10n - 4)x^2 + 6nx.$$

Proof Suppose that u and v are two vertices of L_n and let $d(u, v) = k$. For $k = 1$, there are $2n + 4$ of vertices u, v with $\deg(u) = \deg(v) = 2$, there are $4(n - 1)$ pair of vertices u, v with $\deg(u) = 2$ and $\deg(v) = 4$. So the coefficient of x is $6n$. For $k = 2$, there are $6n$ pair of vertices u, v with $\deg(u) = \deg(v) = 2$, and there are $4(n - 1)$ pair of vertices such as u, v with $\deg(u) = 2$ and $\deg(v) = 4$. So the coefficient of x^2 is $10n - 4$. For $k = 3$, there are $10(n - 1) + 2$ pair of vertices u, v with $\deg(u) = \deg(v) = 2$, there are two pair of vertices u, v with $\deg(u) = 2$ and $\deg(v) = 4$ and $n - 2$ pair of vertices such as u, v with $\deg(u) = \deg(v) = 4$. So the coefficient of x^3 is $11n - 8$.

For $k = 3s + 1$ ($1 \leq s \leq n - 2$) there are $4(n - s + 1)$ pair of vertices u, v with $\deg(u) = \deg(v) = 2$, there are $4(n - s - 1)$ pair of vertices u, v with $\deg(u) = 2$ and $\deg(v) = 4$. So the coefficient of x^{3s+1} ($1 \leq s \leq n - 2$) is $8(n - s)$.

For $k = 3s + 2$ ($1 \leq s \leq n - 2$), there are $4(n - s)$ pair of vertices u, v with $\deg(u) = \deg(v) = 2$, there are $4(n - s - 1)$ pair of vertices u, v with $\deg(u) = 2$ and $\deg(v) = 4$. So the coefficient of x^{3s+2} is $(8n - 8s - 4)$. For $k = 3s$ ($2 \leq s \leq n - 1$) there are $8(n - s)$ pair of vertices u, v with $\deg(u) = \deg(v) = 2$, there are two pairs of vertices such as u, v with $\deg(u) = 2$ and $\deg(v) = 4$, and $n - s - 1$ pair of vertices such as u, v with $\deg(u) = \deg(v) = 4$. So the coefficient of x^{3s} ($2 \leq s \leq n - 1$) is $9n - 9s + 1$.

For $k = 3n - 2$, there are eight pairs of vertices u, v with $\deg(u) = \deg(v) = 2$. For $k = 3n - 1$ and $k = 3n$, there are four and one pair of vertices, respectively. Therefore we have the result. \square

The following corollary gives the Wiener index of L_n .

COROLLARY 3.2 The Wiener index of the para-chain hexagonal cactus graph L_n ($n \geq 3$) is equal to

$$98n - 52 + \sum_{s=1}^{n-2} [(24s + 8)(n - s) + (3s + 2)(8n - 8s - 4)] + \sum_{s=2}^{n-1} 3s(9n - 9s + 1).$$

THEOREM 3.3 The Hosoya polynomial of the para-chain hexagonal cactus graph M_n ($n \geq 4$) is

$$H(M_n, x) = x^{2n+2} + 4x^{2n+1} + 10x^{2n} + 16x^{2n-1} + \sum_{s=3}^{n-1} (13n - 13s + 10)x^{2s} + \sum_{s=2}^{n-2} (12n - 12s + 4)x^{2s+1} + (12n - 16)x^4 + (11n - 8)x^3 + (8n - 2)x^2 + 6nx.$$

Proof Suppose that u and v are two vertices of O_n and let $d(u, v) = k$. For $k = 1$ there are $2n + 4$ vertices u, v with $\deg(u) = \deg(v) = 2$ and $4(n - 1)$ pair of vertices with $\deg(u) = 2$ and $\deg(v) = 4$. So the coefficient of x is $6n$. For $k = 2$ there are $5n$ pair of vertices u, v with $\deg(u) = \deg(v) = 2$, there are $2n$ pair of vertices u, v with $\deg(u) = 2$ and $\deg(v) = 4$, and $n - 2$ pair of vertices such as u, v with $\deg(u) = \deg(v) = 4$. So the coefficient of x^2 is $8n - 2$. For $k = 3$ there are $5n + 2$ pair of vertices u, v with $\deg(u) = \deg(v) = 2$ and $6n - 10$ pair of vertices u, v with $\deg(u) = 2$ and $\deg(v) = 4$. So the coefficient of x^3 is $11n - 8$. For $k = 4$, there are $9(n - 1) - 2$ pair of vertices u, v with $\deg(u) = \deg(v) = 2$, there are $2(n - 1)$ pair of vertices u, v with $\deg(u) = 2$ and $\deg(v) = 4$ and $n - 3$ pair of vertices such as u, v with $\deg(u) = \deg(v) = 4$. So the coefficient of x^4 is $12n - 16$.

For $k = 2s + 1$ ($2 \leq s \leq n - 2$) there are $6(n - s + 1) + 2$ pairs of vertices u, v with $\deg(u) = \deg(v) = 2$, and $6(n - s - 1) + 2$ pairs of vertices u, v with $\deg(u) = 2$ and $\deg(v) = 4$. So the coefficient of x^{2s+1} ($2 \leq s \leq n - 2$) is $(12n - 12s + 4)$.

For $k = 2s$ ($3 \leq s \leq n - 1$) there are $10(n - s + 1) - 1$ pair of vertices u, v with $\deg(u) = \deg(v) = 2$, there are $2(n - s + 1)$ pair of vertices u, v with $\deg(u) = 2$ and $\deg(v) = 4$ and $n - s - 1$ pair of vertices such as u, v with $\deg(u) = \deg(v) = 4$. the coefficient of x^{2s} ($3 \leq s \leq n - 1$) is $(13n - 13s + 10)$.

For $k = 2n - 1$ there are 14 pairs of vertices u, v with $\deg(u) = \deg(v) = 2$, and two pairs of vertices u, v with $\deg(u) = 2$ and $\deg(v) = 4$. So the coefficient of x^{2n-1} is 16. For $k = 2n, k = 2n + 1$ and $k = 2n + 2$, there are ten, four, and one pair of vertices. Therefore we have the result. \square

The following corollary gives the Wiener index of M_n .

COROLLARY 3.4 The Wiener index of the Para-chain hexagonal cactus graph M_n ($n \geq 4$) is equal to

$$165n - 102 + \sum_{s=2}^{n-2} (2s + 1)(12n - 12s + 4) + \sum_{s=3}^{n-1} 2s(13n - 13s + 10).$$

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Author details

Ali Sadeghieh¹

E-mail: sadeghieh@iauyazd.ac.ir

Saeid Alikhani²

E-mail: alikhani@yazd.ac.ir

Nima Ghanbari²

E-mail: n.ghanbari.math@gmail.com

Abdul Jalil M. Khalaf³

E-mail: abduljaleel.khalaf@uokufa.edu.iq

ORCID ID: <http://orcid.org/0000-0002-2447-6666>

¹ Department of Mathematics, Islamic Azad University, Yazd Branch, Yazd, Iran.

² Department of Mathematics, Yazd University, Yazd 89195-741, Iran.

³ Faculty of Computer Science and Mathematics, University of Kufa, P.O. Box 21, Najaf, Iraq.

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