CREAT. MATH. INFORM.
Volume **30** (2021), No. 2,
Pages 181 - 188

Online version at https://creative-mathematics.cunbm.utcluj.ro/
Print Edition: ISSN 1584 - 286X; Online Edition: ISSN 1843 - 441X
DOI: https://doi.org/10.37193/CMI.2021.02.08

Special issue "30 years of publication of CMI

Several Zagreb indices of double square snake graphs

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ABSTRACT. Several lattice structures which can also be thought as graphs are useful in the study of large networks. A recently defined and studied class of such networks are snake graphs. Following the works on square snake graphs, in this work, we study 15 topological graph indices from the class of Zagreb indices of some interesting lattice structures called as double square snake graphs. We use vertex and edge partitions of these graphs and calculate their indices by means of these partitions.

1. SIGNIFICANCE OF THE WORK

In number theory and approximation theory, infinite continued fractions are frequently used to solve several problems such as Pell equations, Diophantine equations, approximating to real numbers, etc. A recently defined graph structure called the square snake graphs are used to study several properties of continued fractions by means of graph methods. In this work, we study several Zagreb-type topologic graph indices of double square snake graphs. We use edge and vertex partitions of the given graphs to calculate the required indices.

2. INTRODUCTION

Snake graphs are studied in different contexts in mathematics and other sciences. They have finite or infinite one or two dimensional repetitions of some geometric shape. They are planar bipartite graphs. Labeling of a graph is a very important subject in graph theory which is done by attaching symbols like integers, letters, etc. according to some rule. Graph labeling can be used in many areas of science where graphs are used to model real life situations. In [12], some snake graphs for square difference prime labelings have been characterized and in [14], difference perfect square cordial labeling of snake graphs have been studied. Similarly, mean sum square prime labeling of snake graphs have been studied in [13]. So, snake graphs are important in the labeling of graphs.

Another important application of snake graphs is number theory. In [3, 4, 5], the authors studied snake graphs in relation with cluster algebras. In [11], Shiffler constructed snake graphs consisting of square tiles and studied them in relation with perfect matchings and positive continued fractions which are used in estimating real numbers by some infinite sequences of rational numbers. Therefore the idea of continued fractions have been a popular and useful area of number theory. They are used in the solutions of some Diophantine equations. Bradshaw et al. continued the above work in [2] and established their relations with linear algebra by studying their characteristic polynomials in relation with the Chebycheff polynomials of the first and second type. In [8], snake graphs are

Received: 17.04.2021. In revised form: 01.06.2021. Accepted: 08.06.2021
2010 *Mathematics Subject Classification.* 05C07, 05C30, 05C38.
Key words and phrases. *Zagreb index, vertex degrees, graph index, square snake graphs, double square snake graphs.*
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studied in relation with strongly *-graphs.

The Zagreb indices, defined nearly 50 years ago in [10], of square snake graphs have been recently studied in [9], see Fig. 1. In this work, we consider double square snake graphs given in Fig. 2.

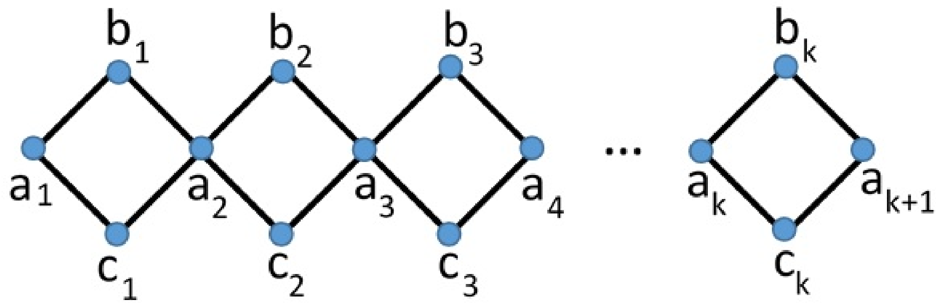

Figure 1 The square snake graph $C^1_{4,k}$

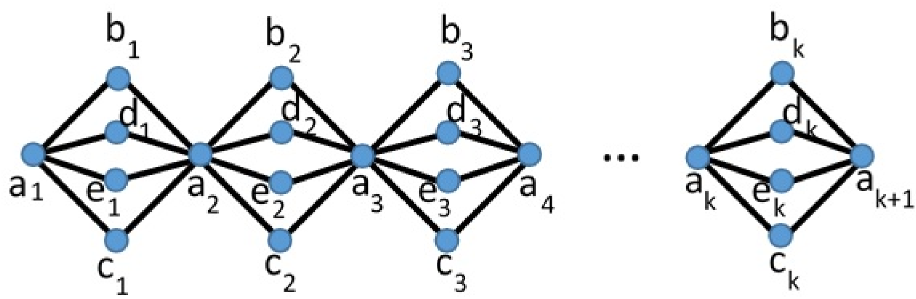

Figure 2 The double square snake graph $D(C^1_{4,k})$

Recent applications of graphs include modeling by graphs. Many real life cases can be modeled by a graph. For example, a chemical molecule can be modeled by a graph in the following way: A vertex is taken for each atom in the molecule and an edge is taken for each chemical bond between two atoms. A graph constructed in such a way is called a molecular or chemical graph. In Chemistry, QSAR and QSPR studies are undertaken by means of several mathematical formulae. A topological index is a mathematical formula calculated by means of either vertex degrees, distances, graph matrices or some graph parameters. They are used to obtain a mathematical value corresponding to a given graph and commenting on such values, one can obtain physico-chemical properties of the corresponding molecules. Modeling by graphs can also be used in other areas of science, especially in network studies and social sciences where there are relations between objects. There are several classes of topological graph indices including Zagreb indices, atom-bond-connectivity indices, geometric-arithmetic indices, Randic indices etc. In this paper, we determine some Zagreb-type topological graph indices of the double square snake graphs $D(C^1_{4,k})$.

3. Some topological indices of double square snake graphs

In this section, we will determine some of the topological graph indices of the double square snake graphs $D(C^1_{4,k})$. The following indices are used in this work:

The first and second Zagreb indices defined by Gutman and Trinajstic, [7], in 1972 are
$M_1(G) = \sum_{v\in V(G)} d_G(v)^2$ and $M_2(G) = \sum_{uv\in E(G)} d_G(u)d_G(v)$.
The total π-electron energy depends on the degree based sums $M_1(G)$ and

$$F(G) = \sum_{u\in V(G)} d_G^3(u).$$

The first index, as we have already seen, is the first Zagreb index and the second sum has never been further studied. In a recent paper, this sum was named as the forgotten index by Furtula and Gutman, [6], and it was shown to have an exceptional applicative potential. In [1], the forgotten index together with the sigma index are calculated for the subdivision and r-subdivision graphs.

The generalized first and second Zagreb indices are defined by

$$M_1^\alpha(G) = \sum_{v\in V(G)} d_G(v)^\alpha$$

and

$$M_2^\alpha(G) = \sum_{uv\in E(G)} (d_G(u)d_G(v))^\alpha.$$

The generalized sum connectivity index is defined by

$$H_\alpha(G) = \sum_{uv\in E(G)} (d_G(u)+d_G(v))^\alpha.$$

The redefined first, second and third Zagreb indices are

$$ReZG_1(G) = \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{d_G(u)d_G(v)},$$

$$ReZG_2(G) = \sum_{uv\in E(G)} \frac{d_G(u)d_G(v)}{d_G(u)+d_G(v)}$$

and

$$ReZG_3(G) = \sum_{uv\in E(G)} d_G(u)d_G(v)(d_G(u)+d_G(v)).$$

The last index is also named as the Gutman index in some sources.
The second Gourava index is defined by

$$M_{r,s}(G) = \sum_{u,v\in E(G)} [d(u)^r.d(v)^s + d(u)^s.d(v)^r].$$

The reformulated first, second Zagreb indices and reformulated forgotten index are defined by

$$RM_1(G) = \sum_{u,v\in E(G)} [d(uv)^2],$$

$$RM_2(G) = \sum_{e,e'\in E(G)} [d_G(e)\cdot d_G(e')]$$

and

$$RF(G) = \sum_{u,v\in E(G)} [d(uv)^3].$$

Finally, the multiplicative first and second Zagreb indices are defined by

$$\prod_1(G) = \prod_{v \in V(G)} d(v)^2$$

and

$$\prod_2(G) = \prod_{u,v \in E(G)} d(u) \cdot d(v).$$

Before determining the above topological graph indices of Zagreb type for the double square snake graphs, we must determine the vertex and edge partitions of the double square snake graph $D(C^1_{4,k})$. It has $5k+1$ vertices and $8k$ edges. The vertex degrees are 2, 4 or 8 and the vertex partition of $D(C^1_{4,k})$ together with the parity of each number is therefore appears as in Table 1:

TABLE 1. Vertex partition of $D(C^1_{4,k})$

d_i	$\sharp\ d_i$
2	$4k$
4	2
8	$k-1$

Similarly, the edge partition of $D(C^1_{4,k})$ together with the parity of each edge type is shown in Table 2:

TABLE 2. Edge partition of $D(C^1_{4,k})$

(d_i, d_j)	$\sharp\ (d_i, d_j)$
(2,4)	8
(2,8)	$8(k-1)$

Now, we are ready to determine the above given Zagreb-type topological graph indices of the double square snake graph $D(C^1_{4,k})$ as follows:

4. MAIN RESULTS

In this section, we shall determine some of the Zagreb-type topological graph indices of the double square snake graphs. We shall be using the vertex and edge partitions of these graphs given in Tables 1 and 2. The results obtained here can be commented to obtain information on several chemical properties of the corresponding molecular structures.

Theorem 4.1. *Some Zagreb-type indices of double square snake graph $D(C^1_{4,k})$ are as follows:*

$$\begin{aligned}
M_1(D(C^1_{4,k})) &= 16(5k-2),\\
M_2(D(C^1_{4,k})) &= 64(2k-1),\\
\prod_1(D(C^1_{4,k})) &= 2^{14k+2},\\
\prod_2(D(C_{4,n})) &= 2^{8(4k-1)},\\
F(D(C^1_{4,k})) &= 32(17k-12),\\
M_1^{\alpha}(D(C^1_{4,k})) &= 2^{\alpha}(4k+2^{\alpha+1}+(k-1)\cdot 2^{2\alpha}),\\
M_2^{\alpha}(D(C^1_{4,k})) &= 2^{3\alpha+3}+(k-1)\cdot 2^{4\alpha+3},\\
H_{\alpha}(D(C^1_{4,k})) &= 8\cdot 6^{\alpha}+8(k-1)\cdot 10^{\alpha},\\
ReZG_1(D(C^1_{4,k})) &= 5k+1,\\
ReZG_2(D(C^1_{4,k})) &= \tfrac{32}{15}(6k-1),\\
ReZG_3(D(C^1_{4,k})) &= 128(10k-7),\\
M_{r,s}(D(C^1_{4,k})) &= 2^{r+s+3}[2^r+2^s+(k-1)(2^{2r}+2^{2s})],\\
RM_1(D(C^1_{4,k})) &= 512k-384,\\
RM_2(D(C^1_{4,k})) &= 1792k-1344,\\
RF(D(C^1_{4,k})) &= 4096k-3584.
\end{aligned}$$

Proof. Let us start with the first Zagreb index. By the definition, using Table 1, we obtain

$$\begin{aligned}
M_1(D(C^1_{4,k})) &= \textstyle\sum_{v\in V(G)} dv^2\\
&= 4k\cdot 2^2+2\cdot 4^2+(k-1)\cdot 8^2\\
&= 16(5k-2).
\end{aligned}$$

Now, using Table 2, we calculate the second Zagreb index of the double square snake graph $D(C^1_{4,k})$. From the edge partition of the double square snake graph in Table 2, we have

$$\begin{aligned}
M_2(D(C^1_{4,k})) &= \textstyle\sum_{uv\in E(G)} du\cdot dv\\
&= 8(2\cdot 4)+8\cdot(k-1)\cdot(2\cdot 8)\\
&= 64(2k-1).
\end{aligned}$$

Let us continue with the first multiplicative Zagreb index. This time, taking the product of the squares of the vertex degrees in Table 1 instead of the sum, we get

$$\begin{aligned}
\prod_1(D(C^1_{4,k})) &= \textstyle\prod_{v\in V(G)} d(v)^2\\
&= 2^{8k}\cdot 2^8\cdot 2^{6k-6}\\
&= 2^{14k+2}.
\end{aligned}$$

The second multiplicative Zagreb index of the double square snake graph is similarly calculated as below:

$$\begin{aligned}\prod_2(D(C^1_{4,k})) &= \prod_{u,v\in E(G)} d(u)\cdot d(v)\\ &= \prod_{v\in V(G)} d(u)^{d(v)}\\ &= 2^{8k}\cdot 4^8\cdot 8^{8(k-1)}\\ &= 2^{8(4k-1)}.\end{aligned}$$

The forgotten Zagreb index of the double square snake graph $D(C^1_{4,k})$ is

$$\begin{aligned}F(D(C^1_{4,k})) &= \sum_{v\in V(G)}(d(v))^3\\ &= 4k\cdot 2^3 + 2\cdot 4^3 + (k-1)\cdot 8^3\\ &= 32(17k-12).\end{aligned}$$

Alternatively, using the edge partition table, we can obtain the same value:

$$\begin{aligned}F(D(C^1_{4,k})) &= \sum_{u,v\in E(G)}[d(u)^2 + d(v)^2]\\ &= 8\cdot(2^2+4^2) + 8(k-1)(2^2+8^2)\\ &= 32(17k-12).\end{aligned}$$

For a real number α, the general first Zagreb index of the double square snake graph $D(C^1_{4,k})$ is

$$\begin{aligned}M_1^\alpha(D(C^1_{4,k})) &= \sum_{v\in V(G)} d(v)^\alpha\\ &= 4k\cdot 2^\alpha + 2\cdot 4^\alpha + (k-1)8^\alpha\\ &= k\cdot 2^{\alpha+2} + 2^{2\alpha+1} + (k-1)2^{3\alpha}.\end{aligned}$$

Also using the edge partition table, we can deduce the same result:

$$\begin{aligned}F(D(C^1_{4,k})) &= \sum_{u,v\in E(G)}[d(u)^{\alpha-1} + d(v)^{\alpha-1}]\\ &= k\cdot 2^{\alpha+2} + 2^{2\alpha+1} + (k-1)2^{3\alpha}.\end{aligned}$$

The general second Zagreb index of the double square snake graph $D(C^1_{4,k})$ is found to be

$$\begin{aligned}M_2^\alpha(D(C^1_{4,k})) &= \sum_{u,v\in E(G)}[d(u)\cdot d(v)]^\alpha\\ &= 8(2\cdot 4)^\alpha + 8(k-1)(2\cdot 8)^\alpha\\ &= 8^{\alpha+1} + (k-1)2^{4\alpha+3}.\end{aligned}$$

The general sum connectivity index of the double square snake graph $D(C^1_{4,k})$ is

$$\begin{aligned}H_\alpha(D(C^1_{4,k})) &= \sum_{u,v\in E(G)}[d(u)+d(v)]^\alpha\\ &= \sum_{u,v\in E(G)}[d(uv)+2]^\alpha\\ &= 8(2+4)^\alpha + 8(k-1)(2+8)^\alpha\\ &= 8\cdot 6^\alpha + 8(k-1)10^\alpha\end{aligned}$$

The redefined first Zagreb index of the double square snake graph $D(C^1_{4,k})$ is

$$\begin{aligned}ReZG_1(D(C^1_{4,k})) &= \sum_{u,v\in E(G)}\\ &= \sum_{u,v\in E(G)}[\tfrac{d(u)+d(v)}{d(u)\cdot d(v)}]\\ &= 8(\tfrac{6}{8}) + 8(k-1)\tfrac{10}{16}\\ &= 5k+1\end{aligned}$$

and the redefined second Zagreb index of the double square snake graph $D(C^1_{4,k})$ is

$$\begin{aligned}ReZG_2(D(C^1_{4,k})) &= \sum_{u,v\in E(G)}[\tfrac{d(u)d(v)}{d(u)+d(v)}]\\ &= 8(\tfrac{8}{6}) + 8(k-1)\tfrac{16}{10}\\ &= \tfrac{32}{3} + \tfrac{64}{5}(k-1)\\ &= \tfrac{32}{15}\cdot(6k-1).\end{aligned}$$

Similarly, the redefined third Zagreb index of the double square snake graph $D(C^1_{4,k})$ would be obtained by

$$\begin{aligned} ReZG_3(D(C^1_{4,k})) &= \sum_{u,v\in E(G)}[d(u)\cdot d(v)]\cdot[d(u)+d(v)] \\ &= (6\cdot 8)\cdot 8+(16\cdot 10)\cdot 8(k-1) \\ &= 128(10k-7). \end{aligned}$$

The second Gourava index of the double square snake graph $D(C^1_{4,k})$ is

$$\begin{aligned} M_{r,s}(D(C^1_{4,k})) &= \sum_{u,v\in E(G)}[d(u)^r\cdot d(v)^s+d(u)^s\cdot d(v)^r], \forall r,s\in R \\ &= 8[2^r\cdot 4^s+2^s\cdot 4^r]+8(k-1)[2^r\cdot 8^s+2^s\cdot 8^r] \\ &= 2^{r+s+3}[2^r+2^s+(k-1)(2^{2r}+2^{2s})]. \end{aligned}$$

Finally, the reformulated first, second and third (forgotten) Zagreb indices of the double square snake graph $D(C^1_{4,k})$ are

$$\begin{aligned} RM_1(D(C^1_{4,k})) &= \sum_{u,v\in E(G)}[d(uv)^2] \\ &= \sum_{u,v\in E(G)}[d(u)+d(v)-2]^2 \\ &= 8[2+4-2]^2+8(k-1)[2+8-2]^2 \\ &= 512k-384; \end{aligned}$$

$$\begin{aligned} RM_2(D(C^1_{4,k})) &= \sum_{e,e'\in E(G)}[d_G(e)\cdot d_G(e^{'})] \\ &= (4\cdot 4)\cdot 12+(4\cdot 8)\cdot 8+(8\cdot 8)\cdot 28(k-1) \\ &= 1792k-1344 \end{aligned}$$

and

$$\begin{aligned} RF(D(C^1_{4,k})) &= \sum_{u,v\in E(G)}[d(uv)^3] \\ &= (2+4-2)^3\cdot 8+(2+8-2)^3\cdot 8(k-1) \\ &= 4096k-3584. \end{aligned}$$

□

5. Results, discussion and applications

The first two Zagreb indices had appeared nearly 50 years ago in the topological study of π-electron energy. They were first used as branching indices which were later called as topological indices. As there are several topological indices which have been used to determine or compare the boiling points of some alkanes such as the Wiener index and first and second Zagreb indices, here we study the class of Zagreb indices to calculate their values for the double square snake graphs. Double square snake graphs are considered as special network structures and their Zagreb-type graph indices are calculated throughly. The values we obtained here can be used to compare the boiling points of corresponding chemical substances and these results can be extended to QSPR studies of other chemical substances. Similar studies can be done for other lattice types and for other topological graph indices.

6. Conclusions

A recent graph type called double square snake graphs and their variants are studied in this manuscript and their Zagreb-type topological graph indices are calculated. These graphs are defined and studied in relation with the continued fractions in number theory. The methods used here can be applied similarly to other similar network structures.

DISCLOSURE STATEMENT

The authors acknowledge that there is no conflict betweeen them and they all equally contributed to the paper. No part of it has been published or simultaneously submitted to any other journals. No potential conflict of interest was reported by the authors.

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