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$(\beta, \alpha)-$Connectivity Index of Graphs

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Abstract

Let $E_\beta(G)$ be the set of paths of length β in a graph G. For an integer $\beta \geq 1$ and a real number α, the (β, α)-connectivity index is defined as

$$^{\beta}\chi_\alpha(G) = \sum_{v_1v_2\cdots v_{\beta+1} \in E_\beta(G)} (d_G(v_1)d_G(v_2)...d_G(v_{\beta+1}))^\alpha.$$

The $(2,1)$-connectivity index shows good correlation with acentric factor of an octane isomers. In this paper, we compute the $(2,\alpha)$-connectivity index of certain class of graphs, present the upper and lower bounds for $(2,\alpha)$-connectivity index in terms of number of vertices, number of edges and minimum vertex degree and determine the extremal graphs which achieve the bounds. Further, we compute the $(2,\alpha)$-connectivity index of line graphs of subdivision graphs of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$, tadpole graphs, wheel graphs and ladder graphs.

Keywords: degree; Zagreb indices; connectivity index; line graph; subdivision graph; nanostructures
AMS 2010 codes: 05C90, 05C35, 05C12

1 Introduction

Let $G = (V,E)$ be a simple graph with $n = |V|$ vertices and $m = |E|$ edges. As usual, n is said to be an order and m the size of G. The subdivision graph $S(G)$ is the graph obtained from G by replacing each edge by a path of length 2. The line graph $L(G)$ of G is the graph whose vertex set is $E(G)$ in which two vertices are adjacent if and only if they are adjacent in G. The tadpole graph $T_{n,k}$ is the graph obtained by joining a cycle of n vertices with a path of length k. The cartesian product $G \times H$ of graphs G and H has the vertex set $V(G \times H) = V(G) \times V(H)$ and $(a,x)(b,y)$ is an edge of $G \times H$ if and only if $[a = b$ and $xy \in E(H)]$ or $[x = y$ and $ab \in E(G)]$. The ladder graph L_n is given by $L_n = K_2 \times P_n$, where P_n is the path of length n. Let $E_\beta(G)$ be the set of paths of length β in G. We refer to [13] for unexplained terminology and notation.

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Chemical graph theory is a branch of mathematical chemistry concerned with the study of chemical graphs. Chemical graphs are models of molecules in which atoms are represented by vertices and chemical bonds by edges of a graph. A graphical invariant is a number related to a graph. In other words, it is a fixed number under graph automorphisms. In chemical graph theory, these invariants are also called the topological indices. The first and second Zagreb indices are defined as

$$M_1(G) = \sum_{u\in V(G)} d_G(u)^2 = \sum_{uv\in E(G)} [d_G(u)+d_G(v)] \text{ and } M_2(G) = \sum_{uv\in E(G)} d_G(u)d_G(v)$$

respectively.

The connectivity index of an organic molecule whose molecular graph G is defined (see [12, 17]) as

$$^1\chi_\alpha(G) = \sum_{uv\in E(G)} (d_G(u)d_G(v))^\alpha.$$

For an integer $\beta \geq 1$ and a real number α, the (β,α)-connectivity index [14] is defined as

$$^\beta\chi_\alpha(G) = \sum_{v_1v_2\cdots v_{\beta+1}\in E_\beta(G)} (d_G(v_1)d_G(v_2)...d_G(v_{\beta+1}))^\alpha. \quad (1)$$

The higher connectivity indices are of great interest in molecular graph theory [15, 22] and some of their mathematical properties have been reported in [1, 18, 19]. Chemical applications of higher connectivity indices are the motivations for our study.

By Eq. (1), it is consistent to define $(2,\alpha)$-connectivity index and $(2,1)$-connectivity index as

$$^2\chi_\alpha(G) = \sum_{uvw\in E_2(G)} (d_G(u)d_G(v)d_G(w))^\alpha \text{ and} \quad (2)$$

$$^2\chi_1(G) = \sum_{uvw\in E_2(G)} (d_G(u)d_G(v)d_G(w)) \quad (3)$$

respectively.

The present paper is organized as follows. In Section 2, we study the chemical applicability of the $(2,1)$-connectivity index. In Section 3, we compute the $(2,\alpha)$-connectivity index of certain class of graphs and present the upper and lower bounds for $(2,\alpha)$-connectivity index in terms of the number of vertices, the number of edges and the minimum vertex degree and determine the extremal graphs which achieve the bounds. In Section 4, we compute the $(2,\alpha)$-connectivity index of line graphs of subdivision graphs of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$, tadpole graphs, wheel graphs and ladder graphs.

2 On the chemical applicability of the $(2,1)$-connectivity index

Octane isomers have become an important set of organic molecules to test the applicability of various topological parameters in quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR). The productivity of $(2,1)$-connectivity index was tested using a dataset of octane isomers, found at http://www.moleculardescriptors.eu/dataset.htm. It is shown that the $(2,1)$-connectivity index has a good correlation with the acentric factor of an octane isomers.

The dataset of octane isomers (first two columns of Table 1) are taken from http://www.moleculardescriptors.eu/dataset.htm and the last column of Table 1 is computed from the definition of $(2,1)$-connectivity index.

The linear regression model for the acentric factor of Table 1 is obtained by using the least squares fitting procedure as implemented in $R-$software [24]. The fitted model is

$$AcentFac = 0.4547376 - 0.0016125\,{}^2\chi_1$$

Table 1 Experimental values of the acentric factor and corresponding values of $^2\chi_1$ of octane isomers.

Alkane	AcentFac	$^2\chi_1$
n-octane	0.397898	40
2-methyl-heptane	0.377916	47
3-methyl-heptane	0.371002	54
4-methyl-heptane	0.371504	56
3-ethyl-hexane	0.362472	64
2,2-dimethyl-hexane	0.339426	64
2,3-dimethyl-hexane	0.348247	70
2,4-dimethyl-hexane	0.344223	63
2,5-dimethyl-hexane	0.35683	54
3,3-dimethyl-hexane	0.322596	80
3,4-dimethyl-hexane	0.340345	78
2-methyl-3-ethyl-pentane	0.332433	81
3-methyl-3-ethyl-pentane	0.306899	96
2,2,3-trimethyl-pentane	0.300816	96
2,2,4-trimethyl-pentane	0.30537	75
2,3,3-trimethyl-pentane	0.293177	103
2,3,4-trimethyl-pentane	0.317422	87
2,2,3,3-tetramethylbutane	0.255294	120

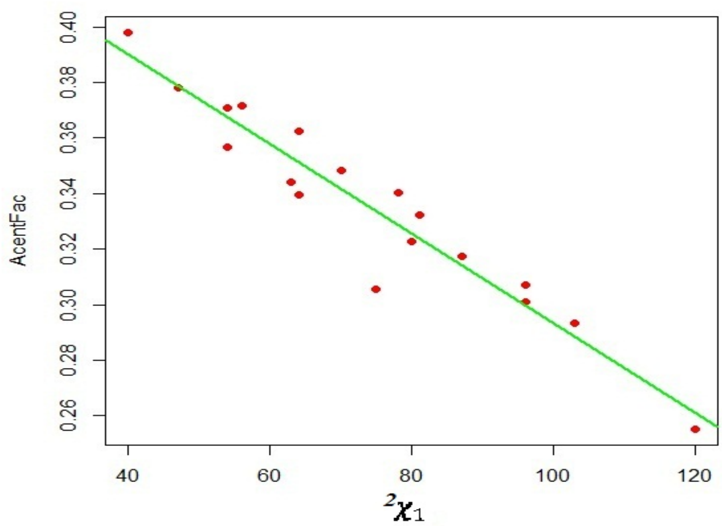

Fig. 1 Scatter diagram of *AcentFac* on $^2\chi_1$, superimposed by the fitted regression line.

The values of $(2,1)$-connectivity index against values of acentric factor of an octane isomers are plotted in Fig. 1. The absolute value of correlation coefficient between AcentFac and $^2\chi_1$ is 0.95802 and with standard error 0.01047.

3 Estimating the $(2,\alpha)$-connectivity index of graphs

We start by stating the following observation, which is needed to prove our main results.

Remark 1. For a graph G on m edges, the number of paths of length 2 in G is $-m+\frac{1}{2}M_1(G)$.

Theorem 1. *For a path P_n on $n>4$ vertices,*

$$^2\chi_\alpha(P_n) = 2\cdot 4^\alpha + 8^\alpha\cdot(n-4)$$

Proof. For a path P_n on $n>4$ vertices each vertex is of degree either 1 or 2. Based on the degree of vertices on the path of length 2 in P_n we can partition $E_2(P_n)$. In P_n, path $(1,2,2)$ appears 2 times and path $(2,2,2)$ appears $(n-4)$ times. Hence by Eq. (2) we get the required result.

Theorem 2. *For a wheel graph W_{n+1},*

$$^2\chi_\alpha(W_{n+1}) = 27^\alpha\cdot n + (9n)^\alpha\cdot\tfrac{n^2+3n}{2}.$$

Proof. For a wheel W_{n+1} on $n\geq 3$ vertices each vertex is of degree either 3 or n. Based on the degree of vertices on the path of length 2 in W_{n+1} we can partition $E_2(W_{n+1})$. In W_{n+1}, path $(3,3,3)$ appears n times and path $(3,3,n)$ appears $\frac{n^2+3n}{2}$ times. Therefore by Eq. (2), we get the required result.

Theorem 3. *For a complete bipartite graph $K_{r,s}$,*

$$^2\chi_\alpha(K_{r,s}) = \tfrac{r^{2\alpha+1}\cdot s^{\alpha+1}\cdot(s-1)}{2} + \tfrac{r^{\alpha+1}\cdot s^{2\alpha+1}\cdot(r-1)}{2}$$

Proof. For a complete bipartite graph $K_{r,s}$ on $r+s$ vertices each vertex is of degree either r or s. Based on the degree of vertices on the path of length 2 in $K_{r,s}$ we can partition $E_2(K_{r,s})$. In $K_{r,s}$, path (r,s,r) appears $\frac{rs(s-1)}{2}$ times and path (s,r,s) appears $\frac{sr(r-1)}{2}$ times. Hence by Eq. (2), we get the required result.

Theorem 4. *Let G be a r-regular graph on n vertices,*

$$^2\chi_\alpha(G) = r^{3\alpha+1}\cdot\tfrac{n(r-1)}{2}.$$

Proof. Since G is a r-regular graph, the path (r,r,r) appears $\frac{nr(r-1)}{2}$ times in G. Therefore by Eq. (2), we get the required result.

Corollary 5. *For a cycle C_n, $^2\chi_\alpha(C_n) = 8^\alpha\cdot n$.*

Corollary 6. *For a complete graph K_n, $^2\chi_\alpha(K_n) = \frac{n(n-2)\cdot(n-1)^{3\alpha+1}}{2}$.*

Lemma 7 (c.f. [3])**.** *Let G be a graph with n vertices and m edges. Then*

$$M_1(G) \leq m(\frac{2m}{n-1}+n-2). \tag{4}$$

Lemma 8 (c.f. [4])**.** *Let G be a graph with n vertices and m edges, $m>0$. Then the equality*

$$M_1(G) = m(\frac{2m}{n-1}+n-2)$$

holds if and only if G is isomorphic to star graph S_n or K_n or $K_{n-1}\cup K_1$.

Theorem 9. *Let G be a graph with n vertices and m edges. Then*

$$^2\chi_1(G) \leq (n-1)^{3\alpha}\cdot m(\frac{m}{n-1}+\frac{n-4}{2}) \tag{5}$$

the equality holds if and only if G is isomorphic to K_n.

Proof.

$$
\begin{aligned}
{}^2\chi_\alpha(G) &= \sum_{uvw\in E_2(G)} [d_G(u)d_G(v)d_G(w)]^\alpha \\
&\leq \sum_{uvw\in E_2(G)} (n-1)^{3\alpha} \qquad (6)\\
&= (n-1)^{3\alpha}(-m+\frac{1}{2}M_1(G)) \\
&\leq (n-1)^{3\alpha}(-m+\frac{1}{2}m(\frac{2m}{n-1}+n-2)) \qquad (7)\\
&= (n-1)^{3\alpha}\cdot m(\frac{m}{n-1}+\frac{n-4}{2}).
\end{aligned}
$$

Relations (6) and (7) were obtained by taking into account for each vertices $v\in V(G)$, we have $d_G(v)\leq n-1$ and Eq. (4), respectively.
Suppose that equality in (5) holds. Then inequalities (6) and (7) become equalities. From (6) we conclude that for every vertex v, $d_G(v) = n-1$. Then from Eq. (7) and Lemma 8 it follows that G is a complete graph.
Conversely, let G be a complete graph. Then it is easily verified that equality holds in (5).

Lemma 10 (c.f. [4])**.** *Let G be a graph with n vertices and m edges. Then*

$$M_1(G)\geq 2m(2p+1)-pn(1+p),\ \textit{where}\ p=\lfloor\frac{2m}{n}\rfloor,$$

and the equality holds if and only if the difference of the degrees of any two vertices of graph G is at most one.

Theorem 11. *Let G be a graph with n vertices, m edges and the minimum vertex degree δ. Then*

$$ {}^2\chi_\alpha(G)\geq \frac{\delta^{3\alpha}}{2}(4mp-pn(p+1)),\ \textit{where}\ p=\lfloor\frac{2m}{n}\rfloor, \qquad (8)$$

and the equality holds if and only if G is a regular graph.

Proof.

$$
\begin{aligned}
{}^2\chi_\alpha(G) &= \sum_{uvw\in E_2(G)} [d_G(u)d_G(v)d_G(w)]^\alpha \\
&\geq \sum_{uvw\in E_2(G)} \delta^{3\alpha} \qquad (9)\\
&= \delta^{3\alpha}(-m+\frac{1}{2}M_1(G)) \\
&\geq \delta^{3\alpha}(-m+\frac{1}{2}(2m(2p+1)-pn(1+p))) \qquad (10)\\
&= \frac{\delta^{3\alpha}}{2}(4mp-pn(p+1)).
\end{aligned}
$$

Relations (9) and (10) were obtained by taking into accounting for each vertices $v\in V(G)$, we have $d_G(v)\geq\delta$ and Eq. (8), respectively.
Suppose now that equality in (8) holds. Then inequalities (9) and (10) become equalities. From (9) we conclude that for every vertex v, $d_G(v)=\delta$. Then from Eq. (10) and Lemma 10 it follows that G is a regular graph.
Conversely, let G be a regular graph. Then it is easily verified that equality holds in (8).

4 Computing the $(2,\alpha)$-connectivity index of line graphs of subdivision graphs of some families of graphs

In [16], Nadeem et al. obtained expressions for certain topological indices of the line graphs of subdivision graphs of 2D-lattice, nanotube, and nanotorus of $TUC_4C_8[p,q]$, where p and q denote the number of squares in a row and the number of rows of squares, respectively in 2D-lattice, nanotube and nanotorus as shown in Figure 2 (a), (b) and (c)respectively. The numbers of vertices and edges of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$ are given in Table 2. Readers interested in other information on nanostructures can be referred to [2, 5–9, 11].

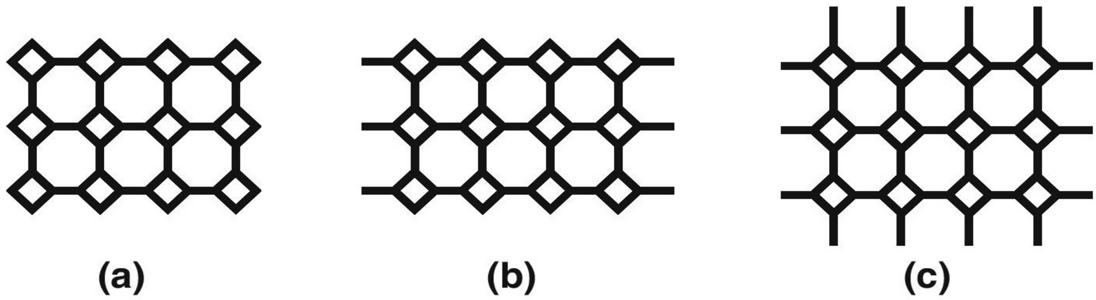

Fig. 2 (a) 2D-lattice of $TUC_4C_8[4,3]$; (b) $TUC_4C_8[4,3]$ nanotube; (c) $TUC_4C_8[4,3]$ nanotorus.

Table 2 Number of vertices and edges.

Graph	Number of vertices	Number of edges
2D-lattice of $TUC_4C_8[p,q]$	$4pq$	$6pq-p-q$
$TUC_4C_8[p,q]$ nanotube	$4pq$	$6pq-p$
$TUC_4C_8[p,q]$ nanotorus	$4pq$	$6pq$

In [20, 21], Ranjini et al. presented explicit formula for computing the Shultz index and Zagreb indices of the subdivision graphs of the tadpole, wheel and ladder graphs. In 2015, Su and Xu [23] calculated the general sum-connectivity index and coindex of the $L(S(T_{n,k}))$, $L(S(W_n))$ and $L(S(L_n))$. In [11], Nadeem et al. derived some exact formulas for ABC_4 and GA_5 indices of the line graphs of the tadpole, wheel and ladder graphs by using the notion of subdivision.

Table 3 Partition of paths of length 2 of the graph X.

$(d_X(u),d_X(v),d_X(w))$ where $uvw \in E_2(X)$	$(2,2,2)$	$(2,2,3)$	$(3,3,2)$	$(3,3,3)$
Number of paths of length 2 in X	8	$4(p+q-2)$	$8(p+q-2)$	$(36pq-26p-26q+16)$

Lemma 12 (c.f. [16]). *Let X be the line graph of the subdivision graph of 2D-lattice of $TUC_4C_8[p,q]$. Then $M_1(X)=108pq-38p-38q$.*

Theorem 13. *Let X be the line graph of the subdivision graph of 2D-lattice of $TUC_4C_8[p,q]$. Then ${}^2\chi_\alpha(X)=8^{\alpha+1}+4(12^\alpha+2\cdot 18^\alpha)(p+q-2)+27^\alpha(36pq-26p-26q+16)$.*

Proof. The subdivision graph of 2D-lattice of $TUC_4C_8[p,q]$ and the graph X are shown in Fig.3 (a) and (b),

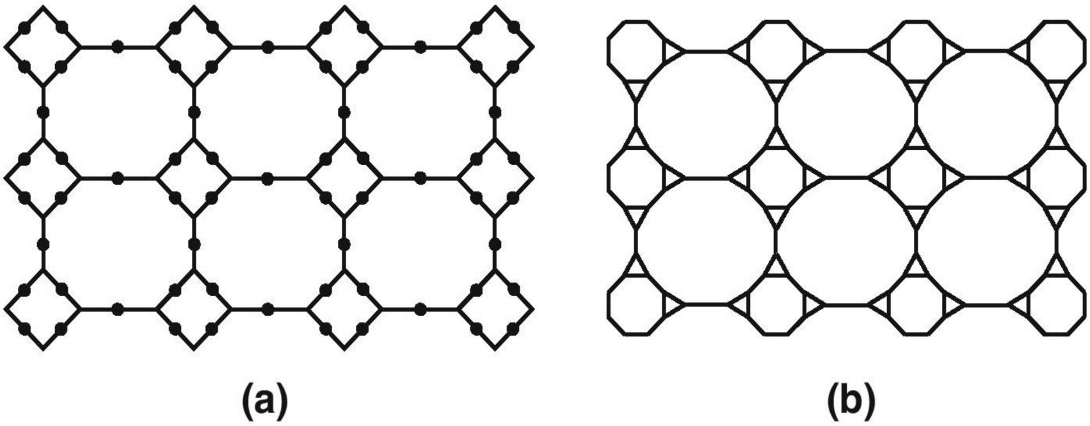

Fig. 3 (a) Subdivision graph of 2D-lattice of $TUC_4C_8[4,3]$; (b) Line graph of the subdivision graph of 2D-lattice of $TUC_4C_8[4,3]$.

respectively. In X there are total $2(6pq-p-q)$ vertices each vertex is of degree either 2 or 3 and $18pq-5p-5q$ edges. From Observation 1 and Lemma 12, we get $36pq-14p-14q$ of paths of length 2 in X. Based on the degree of vertices on the path of length 2 in X we can partition $E_2(X)$ as shown in Table 3. Apply Eq. (2) to Table 3 and get the required result.

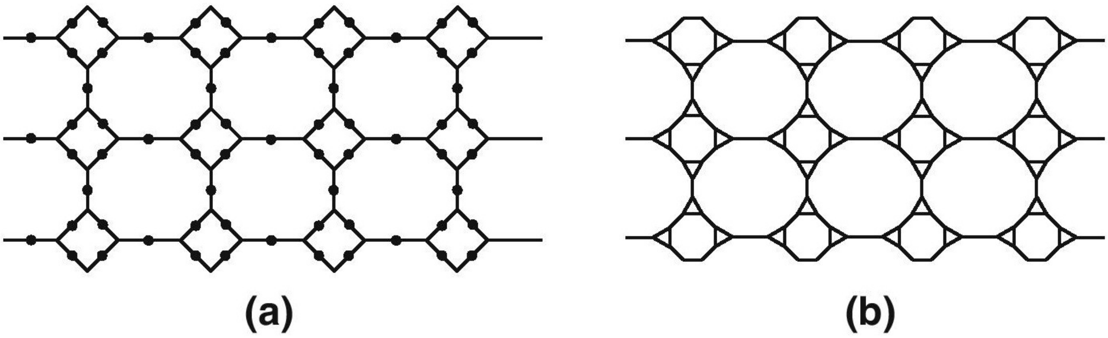

Fig. 4 (a) Subdivision graph of $TUC_4C_8[4,3]$ of nanotube; (b) line graph of the subdivision graph of $TUC_4C_8[4,3]$ of nanotube.

Table 4 Partition of paths of length 2 of the graph Y.

$(d_Y(u),d_Y(v),d_Y(w))$ where $uvw\in E_2(Y)$	$(2,2,3)$	$(3,3,2)$	$(3,3,3)$
Number of paths of length 2 in Y	$4p$	$8p$	$(36pq-26p)$

Lemma 14 (c.f. [16]). *Let Y be the line graph of the subdivision graph of $TUC_4C_8[p,q]$ nanotube. Then $M_1(Y)$=$108pq-38p$.*

Theorem 15. *Let Y be the line graph of the subdivision graph of $TUC_4C_8[p,q]$ nanotube. Then $^2\chi_\alpha(Y)=12^\alpha\cdot 4p+18^\alpha\cdot 8p+27^\alpha(36pq-26p)$.*

Proof. The subdivision graph of $TUC_4C_8[p,q]$ nanotube and the graph Y are shown in Fig.4 (a) and (b), respectively. In Y there are total $12pq-2p$ vertices in which each vertex is of degree either 2 or 3 and $18pq-5p$ edges. From Remark 1 and Lemma 14, we get $36pq-14p$ number of paths of length 2 in Y. Based on the degree of vertices on the paths of length 2 in Y we can partition $E_2(Y)$ as shown in Table 4. Apply Eq. (2) to Table 4 and get the required result.

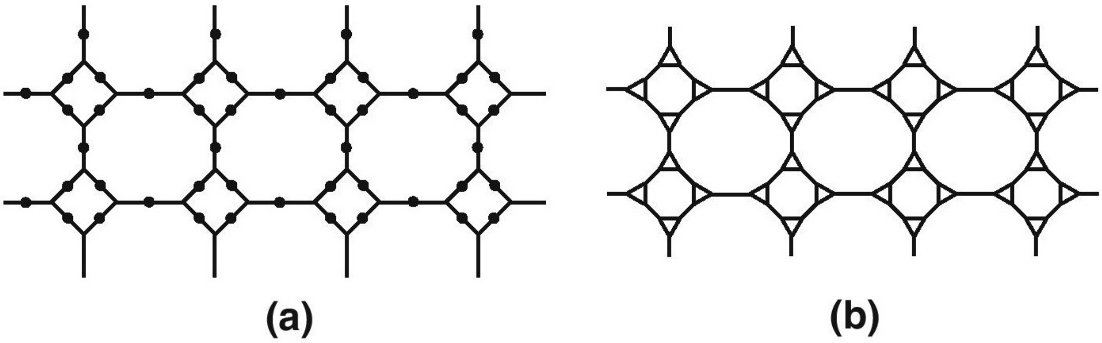

Fig. 5 (a) Subdivision graph of $TUC_4C_8[4,3]$ of nanotorus; (b) Line graph of the subdivision graph of $TUC_4C_8[4,3]$ of nanotorus.

Theorem 16. *Let Z be the line graph of the subdivision graph of $TUC_4C_8[p,q]$ nanotorus. Then $^2\chi_\alpha(Z) = 27^\alpha \cdot 36pq$.*

Proof. The subdivision graph of $TUC_4C_8[p,q]$ nanotorus and the graph Z are shown in Fig.5 (a) and (b), respectively. Since Z is a 3-regular graph with $12pq$ vertices and $18pq$ edges. Therefore by Theorem 4, we get the required result.

Table 5 Partition of paths of length 2 of the graph $A = L(S(T_{n,k}))$ for $k = 1$

$(d_A(u), d_A(v), d_A(w))$ where $uvw \in E_2(A)$	$(1,3,3)$	$(2,3,3)$	$(2,2,3)$	$(3,3,3)$	$(2,2,2)$
Number of paths of length 2 in A	2	4	2	3	$2n-4$

Table 6 Partition of paths of length 2 of the graph $A = L(S(T_{n,k}))$ for $k > 1$

$(d_A(u), d_A(v), d_A(w))$ where $uvw \in E_2(A)$	$(1,2,2)$	$(2,3,3)$	$(2,2,3)$	$(3,3,3)$	$(2,2,2)$
Number of paths of length 2 in A	1	6	3	3	$2n+2k-8$

Lemma 17 (c.f. [20, 23]). *Let A be a line graph of the subdivision graph of the tadpole graph $T_{n,k}$. Then $M_1(A) = 8n+8k+12$.*

Theorem 18. *Let A be a line graph of the subdivision graph of the tadpole graph $T_{n,k}$. Then*

$$^2\chi_\alpha(A) = \begin{cases} 4^\alpha + 18^\alpha \cdot 6 + 12^\alpha \cdot 3 + 27^\alpha \cdot 3 + 8^\alpha \cdot (2n+2k-8) & for\ k > 1. \\ 9^\alpha + 18^\alpha \cdot 4 + 12^\alpha \cdot 2 + 27^\alpha \cdot 3 + 8^\alpha \cdot (2n-4) & for\ k = 1. \end{cases}$$

Proof. First of all, we consider graph A for $n \geq 3$ and $k > 1$. In this graph there are total $2(n+k)$ vertices and $2n+2k+1$ edges. From Remark 1 and Lemma 17, we get $2k+2n+5$ of paths of length 2 in A. Based on the degree of vertices on the paths of length 2 in A we can partition $E_2(A)$ as shown in Table 6. Apply Eq. (2) to Table 6 and get the required result. By similar arguments we can obtain the expression of $^2\chi_\alpha(A)$ for $k = 1$ from Table 5.

Lemma 19 (c.f. [20]). *Let B be a line graph of the subdivision graph of the wheel graph W_{n+1}. Then $M_1(B) = n^3 + 27n$.*

Table 7 Partition of paths of length 2 of the graph B.

$(d_B(u),d_B(v),d_B(w))$ where $uvw \in E_2(B)$	$(3,3,3)$	$(3,3,n)$	$(3,n,n)$	(n,n,n)
Number of paths of length 2 in B	$7n$	$2n$	$n(n-1)$	$\frac{n(n-1)(n-2)}{2}$

Theorem 20. *Let B be a line graph of the subdivision graph of the wheel graph W_{n+1}. Then* $^2\chi_\alpha(B) = 7n\cdot 27^\alpha + n^{\alpha+1}\cdot 9^\alpha \cdot 2 + 3^\alpha \cdot n^{2\alpha+1}(n-1) + n^{3\alpha+1}\cdot \frac{(n-1)(n-2)}{2}$.

Proof. The graph $L(S(W_{n+1}))$ contains $4(n+1)$ vertices and $\frac{n^2+9n}{2}$ edges. From Remark 1 and Lemma 19, we get $\frac{n^3-n^2+18n}{2}$ number of paths of length 2 in B. Based on the degree of vertices on the paths of length 2 in B we can partition $E_2(B)$ as shown in Table 7. Apply Eq. (2) to Table 7 and get the required result.

Table 8 Partition of paths of length 2 of the graph C.

$(d_C(u),d_C(v),d_C(w))$ where $uvw \in E_2(C)$	$(2,2,2)$	$(2,2,3)$	$(2,3,3)$	$(3,3,3)$
Number of paths of length 2 in C	4	4	8	$18n-44$

Lemma 21 (c.f. [20, 23])**.** *Let C be a line graph of subdivision graph of a ladder graph with order n. Then* $M_1(Z) = 54n-76$.

Theorem 22. *Let C be a line graph of subdivision graph of a ladder graph with order n. Then* $^2\chi_\alpha(C) = 8^\alpha\cdot 4 + 12^\alpha \cdot 4 + 18^\alpha \cdot 8 + 27^\alpha(18n-44)$.

Proof. The graph $L(S(L_n))$ contains $6n-4$ vertices and $\frac{18n-20}{2}$ edges. From Remark 1 and Lemma 21, we get $18n-28$ number of paths of length 2 in C. Based on the degree of vertices on the paths of length 2 in C we can partition $E_2(C)$ as shown in Table 8. Apply Eq. (2) to Table 8 and get the required result.

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