Tamap Journal of Mathematics and Statistics
Volume 2017, Article ID 23

Research Article

Computing the *M*-polynomials for 2*D*-Lattice, Nanotube and Nanotorus by operating the semi-total line and point graphs via degree-based indices

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Received:29 November 2017 / Accepted: 28 December 2017

Abstract: The discovery of new nanomaterials adds new dimensions to industry, electronics, pharmaceutical and biological therapeutics. In this article, authors encountered the closed forms *M*-polynomials of nanostructures such 2*D*-lattice, nanotube and nanotorus of $TUC_4C_8[p, q]$ for some degree-based topological indices. These indices are numerical tendency that often depict quantitative structural activity/property/toxicity/relationships and correlate certain physico-chemical properties, such boiling point, stability, and strain energy of the respective nanomaterial.

Keywords: Topological indices, M-polynomials, 2D-lattice, nanotube, nanotorus, semi-total line and semi-total operator.

INTRODUCTION

Nowadays, nanostructures became most fascinated molecular structures. They created many applications in medicine, electronics and computer science (for more information, see [10, 12, 16]).

In chemical graph theory, a molecular graph is conveniently defined as a simple graph (having no loops and multiple edges) in which atoms and chemical bonds between them are represented by vertices and edges, respectively.

A graph $G = (V, E)$ with vertex set $V(G)$ and edge set $E(G)$ is connected if there is a path between any pair of vertices in G. The degree d_u of a vertex u is the number of edges that are incident to u.

Similarly to the classical total graph *T (G)* of a graph *G*, the semi-total (line) graph $T_1(G)$ of *G* is defined to be the graph whose vertex set is *V (G)U E(G)* where two vertices of $T_1(G)$ are adjacent if and only if (i) they are adjacent edges of *G* or (ii) one is a vertex of *G* and the other is an edge of *G* incident to that vertex. Also the semi-total (point) graph $T_2(G)$ of *G* is defined to be the graph whose vertex set is *V (G) U E(G)* where two vertices of $T_2(G)$ are adjacent if and only if (i) they are adjacent vertices of *G* or (ii) one is a vertex of *G* and the other is an edge of *G* incident to that vertex (for more graph operations, see [11,15,17]).

Chemoinformatics is another emerging field in which quantitative structure-activity (QSAR) and structure-property (QSPR) relationships predict the bio-logical activities and properties of the nanomaterial, [3]. In these studies, some physicochemical properties and topological indices are used to predict bioactivity of the chemical compounds, [19,20]. Algebraic polynomials have also useful applications in chemistry, such as the Hosoya polynomial [6] (also called the Wiener polynomial), which plays a vital role in determining distance-based topological indices. Among other algebraic polynomials, the *M*-polynomials, [2], introduced in 2015, play the same role in determining the closed form of certain degree-based topological indices. The main advantage of *M*-polynomial is the wealth of information that it contains about the degree-based graph invariants.

The aim of this paper is to compute the Zagreb indices, generalized Randic index, inverse Randic index and SDD index, M-polynomials of semi-total (line) graph and semi-total (point) graph of the *2D*-lattice, nanotube and nanotorus of $TUC_4C_8[p, q]$. The construction of these nanostructures is shown in Figure 1.

Let us catalogue all the octagons of $TUC_4C_8[p, q]$ which are just cycles C_8 and all quadrangles C_4 where *p* and *q* denote the number of squares in a row and the number of rows of squares, respectively, as in Figure 2(a). The nanotube is obtained from the lattice by wrapping it up so that each drooping edge from the left-hand side connects to the rightmost vertex of the same row and the nanotorus is obtained from nanotube by wrapping it up so that each drooping edge from the up side connects to the down most vertex of the same column as shown in Figure 2(b) and 2(c).

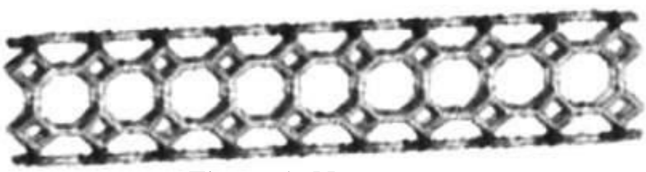

Figure 1: Nanostructure

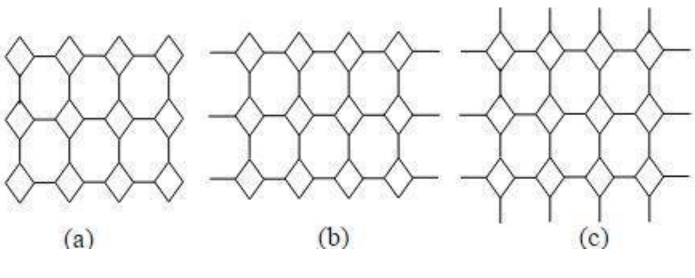

Figure 2: (a) 2*D*-lattice, (b) nanotube, (c) nanotorus

Definition 1: The *M*-polynomial of a graph *G* is defined by

$$M(G,x,y)=\sum_{i\le j} m_{ij}(G)x^i y^j$$

Where $m_{ij}(G)$, $(i, j \geq 1)$, is the number of edges $e = uv$ of *G* such that $(d_u , d_v) = (i, j)$.

Let $AW(G)+BP_3+C$, be the approximated boiling point of alkanes determined by Wiener in 1947, where $W(G)$ is the Wiener index and *A*, *B and C* are empirical constants and P_3 is he number of paths of length 3 in *G* [26]. Thus, Wiener systematizes the support of topological index, which is also known as connectivity index. Many chemical experiments require the conviction of the chemical properties of emanate nanotubes and nanomaterials. Although, no single index in strong enough, out of more than 146 topological indices to determine many physico-chemical properties of a molecule, but the following topological indices can do this to some extent. The Randić index, [18], denoted by $R_{\frac{1}{2}}(G)$ and introduced by Milan Randić in 1975, is also one of the oldest topological indices defined as

$$R_{\frac{1}{2}}(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_u.d_v}},$$

and the generalized Randić index is similarly defined as

$$R_{\alpha}(G)=\sum_{uv\in E(G)}\frac{1}{(d_u.d_v)^{\alpha}}.$$

Finally the inverse Randic index is defined as

$$R'_{\alpha}(G)=\sum_{uv\in E(G)}(d_u.d_v)^{\alpha}.$$

Obviously, $R_{\frac{1}{2}}(G)$ is the particular case of $R_{\alpha}(G)$ when $\alpha=\frac{1}{2}$.

The Randić index is one of the most popular, the most often applied, and the most studied indices amongst all topological indices. Recently, in [14], Lokesha et. al. established some new bounds for Randic index which are quite useful.

Gutman and Trinajstić, [4, 5], introduced the first and second Zagreb indices, which are defined as

$$M_1(G)=\sum_{uv\in E(G)}(d_u+d_v)$$

and

$$M_2(G)=\sum_{uv\in E(G)}d_u.d_v,$$

respectively.

Both the first and second Zagreb indices give greater weights to the inner vertices and edges, and smaller weights to the outer vertices and edges, which opposes intuitive reasoning. For a simple connected graph *G*, the second modified Zagreb index, [8, 25], is defined as

$$^{m}M_2(G)=\sum_{uv\in E(G)}\frac{1}{d_u.d_v}.$$

Recently, D. Vukicević and M. Gasperov, [1, 24], exposed the 148 adriatic indices among which symmetric division deg (*SDD*) index which is defined as

$$SDD(G)=\sum_{uv\in E(G)}\frac{d_u^2+d_u^2}{d_u.d_v},$$

is one of the discrete Adriatic indices, and it has been proved as a good predictor for total surface area for polychlorobiphenyls. Recently, V. Lokesha et.al., [7, 9, 13], worked out *SDD* index of unicyclic and bicyclic graphs which is later extended to tricyclic and tetracyclic graphs. Also this index was calculated for graph operations which gave more attraction to this index.

Table 1 relates some well-known degree-based topological indices with *M*-polynomials.

Table 1: Derivation of some degree-based topological indices from M -polynomials.

Topological indices	$f(x,y)$	*M*-polynomial definitions
$M_1(G)$	$(x+y)$	$\left(D_x+D_y\right)\left(M(G;x,y)\right)\big\|_{x=y=1}$
$M_2(G)$	xy	$\left(D_x.D_y\right)\left(M(G;x,y)\right)\big\|_{x=y=1}$
$^{m}M_2(G)$	$\frac{1}{xy}$	$\left(S_x.S_y\right)\left(M(G;x,y)\right)\big\|_{x=y=1}$
$R'_\alpha(G)$	$(xy)^\alpha$	$\left(D_x^\alpha.D_y^\alpha\right)\left(M(G;x,y)\right)\big\|_{x=y=1}$
$R_\alpha(G)$	$\frac{1}{(xy)^\alpha}$	$\left(S_x^\alpha.S_y^\alpha\right)\left(M(G;x,y)\right)\big\|_{x=y=1}$
$SDD(G)$	$\frac{x^2+y^2}{xy}$	$\left(D_xS_y+S_xD_y\right)\left(M(G;x,y)\right)\big\|_{x=y=1}$

where $D_x=\frac{\partial(f(x,y))}{\partial x}$, $D_y=\frac{\partial(f(x,y))}{\partial y}$, $S_x=\int_0^x\frac{f(t,y)}{t}dt$ and $S_y=\int_0^y\frac{f(x,t)}{t}dt.$

This paper is organized as follows. Section 1 consists of a brief introduction which is essential for the development of main results. Section 2 consists of the first Zagreb, second Zagreb, modified second Zagreb indices, generalized Randic, inverse Randic indices and SDD index of M-polynomials of the 2D-lattice, nanotube and nanotorus of the $TUC_4C_8[p,q]$ using semi-total (line) graph operator and the final section concentrates on the results about the same topological in-dices of the M-polynomials of the 2D-lattice, nanotube and nanotorus of the T UC_4C_8[p; q] using semi-total (point) graph operator.

2. M-polynomials of 2D -lattice, nanotube and nanotorus of *$TUC_4C_8[p, q]$*

In this section, M-polynomials of $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$ are computed from the graph structures under consideration. The results are established by means of the edge partition method.

Theorem 2.1. Let G be the 2D-Lattice of $TUC_4C_8[p,q]$ then

1) $M(G,x,y)=4x^2y^2+4(p+q-2)x^2y^3+(6pq-5(p+q)+4)x^3y^3$
2) $M_1(G)=36pq-10(p+q).$
3) $M_2(G)=21(p^2+q^2)+16(p+q)+6pq(54pq-30(p+q)+7)-16.$
4) ${}^mM_2(G)=4p^2q^2-\frac{1}{9}(p+q-2)^2.$
5) $R_\alpha(G)=[21(p^2+q^2)+16(p+q)+6pq(54pq-30(p+q)+7)-16]^\alpha.$
6) $R'''_\alpha(G)=[4p^2q^2-\frac{1}{9}(p+q-2)^2]^\alpha.$
7) $SDD(G)=4pq[18pq-5(p+q)]+\frac{4}{3}(p+q-2)^2.$

Proof. Let G be the $2D$-lattice of $TUC_4C_8[p,q]$ where p and q are the number of squares in each row and the number of rows, respectively. This graph has $4pq$ vertices and $(6pq-p-q)$ edges. It can be observed from Figure 2(a) that there are three types of edge partitions, i.e.

$$E_{(2,2)}=\{e=uv\in E(G)\,|\,d_u=2,d_v=2\}\rightarrow|E_{(2,2)}|=4$$
$$E_{(2,3)}=\{e=uv\in E(G)\,|\,d_u=2,d_v=3\}\rightarrow|E_{(2,3)}|=4(p+q-2)$$
$$E_{(3,3)}=\{e=uv\in E(G)\,|\,d_u=3,d_v=3\}\rightarrow|E_{(3,3)}|=6pq-5(p+q)+4.$$

Thus, the M-polynomial of the $2D$-lattice of $TUC_4C_8[p,q]$ is

$$\begin{aligned}M(G,x,y)&=\sum_{i\le j}m_{ij}(G)x^iy^j\\&=\sum_{i=j=2}m_{22}(G)x^2y^2+\sum_{2\le 3}m_{23}(G)x^2y^3+\sum_{i=j=3}m_{33}(G)x^3y^3\\&=\sum_{uv\in E_{(2,2)}}m_{22}(G)x^2y^2+\sum_{uv\in E_{(2,3)}}m_{23}(G)x^2y^3+\sum_{uv\in E_{(3,3)}}m_{33}(G)x^3y^3\\&=|E_{(2,2)}|x^2y^2+|E_{(2,3)}|x^2y^3+|E_{(3,3)}|x^3y^3\end{aligned}$$

Now, from M-polynomial equation we compute the following,

$$M(G,x,y)=4x^2y^2+4(p+q-2)x^2y^3+(6pq-5(p+q)+4)x^3y^3$$
$$D_x=8xy^2+[8(p+q-2)]xy^3+[18pq-15(p+q)+12]x^2y^3$$
$$D_x|_{x=y=1}=18pq-7(p+q)+4$$
$$D_y=8x^2y+12(p+q-2)]x^2y^2+(18pq-15(p+q)+12]x^3y^2$$
$$D_y|_{x=y=1}=18pq-3(p+q)-4$$

$$S_x = 2x^2y^2 + 2(p+q-2)]x^2y^3 + 2pq - \frac{5}{3}(p+q) + 4]x^2y^3$$

$$S_x\,|_{x=y=1} = 2pq + \frac{1}{3}(p+q-2)$$

$$S_y = 2x^2y^2 + \frac{4}{3}x^2y^3 + [2pq - \frac{5}{3}(p+q) + 4]x^3y^3$$

$$S_y\,|_{x=y=1} = 2pq - \frac{1}{3}(p+q-2)$$

Hence, applying these results in equation in topological indices definitions, we obtained required results.

Figure 2 shows the 3D plot of the M-polynomial of the 2D-latttice:

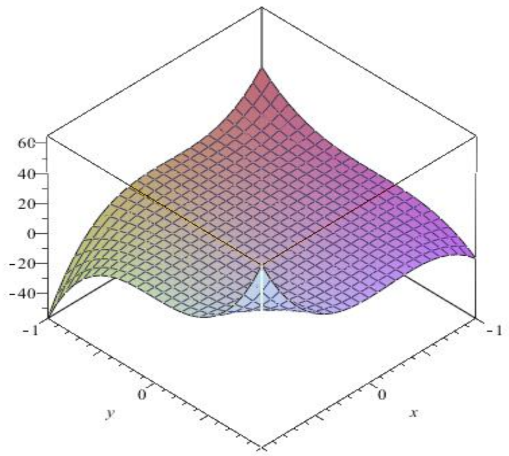

Figure 3: The M-polynomial of 2D-lattice

Theorem 2.2. Let H be the nanotube of *$TUC_4C_8[p,q]$* then

1) $M(H,x,y) = 4px^2y^3 + 6(pq-5p+q)x^3y^3$
2) $M_1(H) = 36pq - 10p + 6q.$
3) $M_2(H) = 6pq(3pq-5) - 36pq(5p-3q) + 3(7p^2+3q^2).$
4) $^{m}M_2(H) = (2pq + \frac{1}{3})^2 - \frac{1}{9}p^2.$
5) $R_\alpha(H) = \{6pq(3pq-5) - 36pq(5p-3q) + 3(7p^2+3q^2)\}^\alpha.$
6) $R'''_\alpha(H) = \left[(2pq + \frac{1}{3})^2 - \frac{1}{9}p^2\right]^\alpha.$
7) $SDD(H) = (18pq - 7p + 3q)\left[2pq + \frac{1}{3}q - \frac{1}{3}p] + [18pq - 3(p+q)][2pq + \frac{1}{3}q + \frac{1}{3}p\right].$

Proof. Let H be the nanotube of *$TUC_4C_8[p,q]$* where p and q are the number of squares in each row and number of rows respectively. This graph has $4pq$ vertices and $(6pq - p + q)$ edges respectively. So, there are two types of edge partitions (Fig. 2(b)), i.e.

$E_{(2,3)} = \{e = uv \in E(H)\,|\,d_u = 2, d_v = 3\} \rightarrow |E_{(2,3)}| = 4p$

$E_{(3,3)} = \{e = uv \in E(H) \mid d_u = 3, d_v = 3\} \rightarrow \mid E_{(3,3)} \mid = 6pq - 5p + q.$

Thus, the M-polynomial of nanotube of *TUC₄C₈[p,q]* is

$$M(H,x,y) = \sum_{i \le j} m_{ij}(H) x^i y^j = \sum_{2 \le 3} m_{23}(H) x^2 y^3 + \sum_{i=j=3} m_{33}(H) x^3 y^3$$
$$= \sum_{uv \in E_{(2,3)}} m_{23}(H) x^2 y^3 + \sum_{uv \in E_{(3,3)}} m_{33}(H) x^3 y^3$$
$$= \mid E_{(2,3)} \mid x^2 y^3 + \mid E_{(3,3)} \mid x^3 y^3$$
$$M(H,x,y) = 4px^2y^3 + (6pq - 5p + q)x^3y^3$$

Hence,

$$D_x = 8pxy^3 + (18pq - 15p + q]x^3y^3$$
$$D_x \mid_{x=y=1} = 18pq - 7p + 3q$$
$$D_y = 12px^2y^2 + (18pq - 5p + q)x^3y^2$$
$$D_y \mid_{x=y=1} = 18pq - 3(p+q)$$
$$S_x = 2px^2y^3 + (2pq - \frac{5}{3}p + \frac{1}{3}q)x^3y^3$$
$$S_x \mid_{x=y=1} = (2pq + \frac{1}{3}q) + \frac{1}{3}p$$
$$S_y = \frac{4}{3}px^2y^3 + (2pq - \frac{5}{3}p + \frac{1}{3}q)x^3y^3$$
$$S_y \mid_{x=y=1} = (2pq + \frac{1}{3}q) - \frac{1}{3}p$$

Since, utilizing these results in topological indices definitions, we get the required results.

Figure 3 shows the M-polynomial of the nanotube of 3D graph:

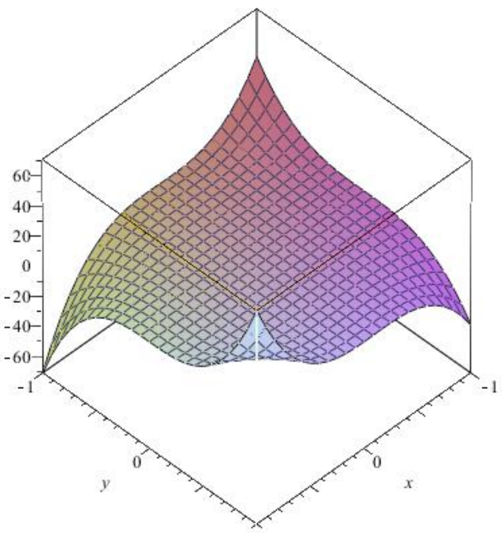

Figure 4: The M-polynomial of Nanotube

Theorem 2.3. Let K be the 2D-Lattice of *$TUC_4C_8[p,q]$* then

1. $M(K,x,y) = (p+q+6pq)x^3y^3$
2. $M_1(K) = 6(6pq+p+q).$
3. $M_2(K) = 9(6pq+p+q)^2.$
4. ${}^mM_2(K) = [\frac{1}{3}(p+q)+2pq]^2.$
5. $R_\alpha(K) = 3(6pq+p+q)^{2^\alpha}.$
6. $R'''_\alpha(K) = [\frac{1}{3}(p+q)+2pq)^{2\alpha}.$
7. $SDD(K) = 2(6pq+p+q)^2.$

Proof. Let K be the nanotorus of *$TUC_4C_8[p,q]$* where p and q are the number of squares in each row and the number of rows, respectively. This graph has $4pq$ vertices and $(6pq + p + q)$ edges, respectively. From Figure 2(c), there is one type of edge partition, i.e.

$E_{(3,3)} = \{e = uv \in E(K) \mid d_u = 3, d_v = 3\} \rightarrow |E_{(3,3)}| = 6pq + p + q.$

$$M(K,x,y) = \sum_{i\le j} m_{ij}(K)x^iy^j = \sum_{i=j=3} m_{33}(K)x^3y^3$$
$$= \sum_{uv\in E_{(3,3)}} m_{33}(K)x^3y^3 = |E_{(3,3)}|\, x^3y^3$$
$$M(K,x,y) = (6pq+p+q)x^3y^3$$
$$\therefore \quad D_x = (3p+3q+18pq)x^2y^3$$
$$D_x|_{x=y=1} = 18pq+3(p+q)$$
$$D_y = (3p+3q+18pq)x^3y^2$$
$$D_y|_{x=y=1} = 18pq+3(p+q)$$
$$S_x = \frac{1}{3}(p+q+6pq)x^3y^3$$
$$S_x|_{x=y=1} = \frac{1}{3}(p+q)+2pq$$
$$S_y = \frac{1}{3}(p+q+6pq)x^3y^3$$
$$S_y|_{x=y=1} = \frac{1}{3}(p+q)+2pq.$$

Thus, by using the table 1, we obtain the essential results.

The following figure 5 shows the 3D graph of the M-polynomial of the nanotorus:

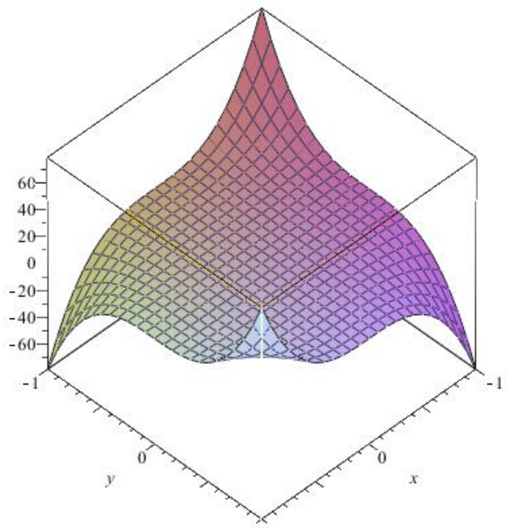

Figure 5: The M-polynomial of the nanotorus

3. Semi-total line graph of $TUC_4C_8[p,q]$

In this section, we compute the closed forms of the *M*-polynomials of the semi-total line graph of the 2*D*-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$ and the structure of the graph depicted in Figure 6.

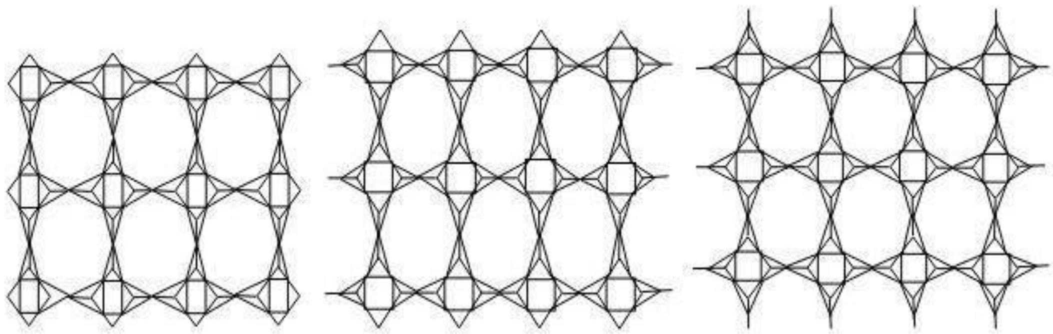

Figure 6: 2*D*-lattice, nanotube, nanotorus graphs of semi-total line graph

Theorem 3.1. Let G_1 be the semi-total line graph of the 2D-lattice of $TUC_4C_8(p, q)$ then,

1) $$M(G_1, x.y) = 8x^2y^4 + [4(p+q)-8]x^2y^5 + [4(p+q)-8]x^3y^5 + [2p(6q-5) + q^2(q-6)+(q+2)]x^3y^6 + (q-2)(q-3)x^4y^4 + [2q(5-q)-4]x^4y^5 + [pq(q-5)+2(4p+q)-8]x^5y^5 + [4(p-q)+4(p+q)(q-1) - (2p+q-1)(q-1)(q-2)]x^5y^6 + \{q(q-1)(5p-6) - (q-1)(q-2)[(p-1)(p-2)+5]\}x^6y^6.$$

2) $M_1(G_1)=2q(4q^2-10q-67)+p(24p-1)+pq(12pq-18p+12q+131)+104.$

3) $$M_2(G_1)=\{8q^2(q-2)+2(7p-26q)+pq(6pq-18p+7q+25)+4(3p^2-4q^2)+104\}\times\{pq(6pq+5q+131)+12(p^2+q^2)-2(20p+41q)\}.$$

4) $${}^{m}M_2(G_1)=\left[pq\left(\frac{1}{2}p+\frac{4}{15}q-\frac{1}{6}pq-\frac{8}{6}\right)-\frac{2}{15}q^3-\frac{1}{3}p^2-\frac{53}{20}q^2+\frac{9}{5}p+\frac{313}{60}q-\frac{68}{15}\right]\times\left[pq\left(\frac{1}{2}p+\frac{7}{10}q-\frac{1}{6}pq\right)+\frac{28}{15}p+\frac{59}{12}q-\frac{1}{3}p^2-\frac{119}{60}q^2-\frac{173}{30}\right].$$

5) $$R_\alpha(G_1)=\{[8q^2(q-2)+2(7p-26q)+pq(6pq-18p+7q+25)+4(3p^2-4q^2)+104[pq(6pq+5q+131)+12(p^2+q^2)-2(20p+41q)]\}^\alpha.$$

6) $$R'_\alpha(G_1)=\left[pq\left(\frac{1}{2}p+\frac{4}{15}q-\frac{1}{6}pq-\frac{8}{6}\right)-\frac{2}{15}q^3-\frac{1}{3}p^2-\frac{53}{20}q^2+\frac{9}{5}p+\frac{313}{60}q-\frac{68}{15}\right]^\alpha\times\left[pq\left(\frac{1}{2}p+\frac{7}{10}q-\frac{1}{6}pq\right)+\frac{28}{15}p+\frac{59}{12}q-\frac{1}{3}p^2-\frac{119}{60}q^2-\frac{183}{30}\right]^\alpha$$

7) $$SDD(G_1)=\{8q^2(q-2)+2(7p-26q)+pq(6pq-18p+7q+25)+4(3p^2-4q^2)+104\}\times\left\{pq\left(\frac{1}{2}p+\frac{7}{10}q-\frac{1}{6}pq+\frac{1}{3}\right)-\frac{p}{15}(5p-28)-\frac{q}{60}(119q-295)-\frac{173}{30}\right\}+\{pq(6pq+5q+131)+12(p^2+q^2)-2(20p+41q)\}\times\left\{pq\left(\frac{1}{2}p+\frac{7}{10}q-\frac{1}{6}pq+\frac{1}{3}\right)-\frac{p}{15}(5p-28)-\frac{q}{60}(119q-295)-\frac{173}{30}\right\}$$

Proof. Let G_1 be the semi-total 2D-lattice of the $TUC_4C_8(p,q)$. The graph has $(10pq-p-q)$ number of vertices and $(24pq-6(p+q))$ number of edges, respectively. By Figure 3, there are nine types of edge partitions,

$E_{(2,4)}=\{e=uv\in E(G_1)|d_u=2,d_v=4\}\rightarrow|E_{(2,4)}|=8$

$E_{(2,5)}=\{e=uv\in E(G_1)|d_u=2,d_v=5\}\rightarrow|E_{(2,5)}|=4(p+q)-8$

$E_{(3,5)}=\{e=uv\in E(G_1)|d_u=3,d_v=5\}\rightarrow|E_{(3,5)}|=4(p+q)-8$

$E_{(3,6)}=\{e=uv\in E(G_1)|d_u=3,d_v=6\}\rightarrow|E_{(3,6)}|=2p(6q-5)+q^2(q-6)+(q+2)$

$E_{(4,4)}=\{e=uv\in E(G_1)|d_u=4,d_v=4\}\rightarrow|E_{(4,4)}|=(q-2)(q-3)$

$E_{(4,5)}=\{e=uv\in E(G_1)|d_u=4,d_v=5\}\rightarrow|E_{(4,5)}|=2q(5-q)-4$

$E_{(5,5)}=\{e=uv\in E(G_1)|d_u=5,d_v=5\}\rightarrow|E_{(5,5)}|=pq(q-5)+2(4p+q)-8$

$E_{(5,6)}=\{e=uv\in E(G_1)|d_u=5,d_v=6\}\rightarrow|E_{(5,6)}|=4(p-q)+4(p+q)(q-1)-(2p+q-1)(q-1)(q-2)$

$E_{(6,6)}=\{e=uv\in E(G_1)|d_u=6,d_v=6\}\rightarrow|E_{(6,6)}|=q(q-1)(5p-6)-(q-1)(q-2)[(p-1)(p-2)+5].$

Thus,

$$
\begin{aligned}
M(G_1,x,y) &= \sum_{i\le j} m_{ij}(G_1)x^i y^j \\
&= \sum_{2\le 4} m_{24}(G_1)x^2y^4 + \sum_{2\le 5} m_{25}(G_1)x^2y^5 + \sum_{3\le 5} m_{35}(G_1)x^3y^5 + \sum_{3\le 6} m_{36}(G_1)x^3y^6 \\
&+ \sum_{i=j=4} m_{44}(G_1)x^4y^4 + \sum_{4\le 5} m_{45}(G_1)x^4y^5 + \sum_{i=j=5} m_{55}(G_1)x^5y^5 + \sum_{5\le 6} m_{56}(G_1)x^5y^6 \\
&+ \sum_{i=j=6} m_{66}(G_1)x^6y^6. \\
&= \sum_{uv\in E_{(2,4)}} m_{24}(G_1)x^2y^4 + \sum_{uv\in E_{(2,5)}} m_{25}(G_1)x^2y^5 + \sum_{uv\in E_{(3,5)}} m_{35}(G_1)x^3y^5 + \sum_{uv\in E_{(3,6)}} m_{36}(G_1)x^3y^6 \\
&+ \sum_{uv\in E_{(4,4)}} m_{44}(G_1)x^4y^4 + \sum_{uv\in E_{(4,5)}} m_{45}(G_1)x^4y^5 + \sum_{uv\in E_{(5,5)}} m_{55}(G_1)x^5y^5 + \sum_{uv\in E_{(5,6)}} m_{56}(G_1)x^5y^6 \\
&+ \sum_{uv\in E_{(6,6)}} m_{66}(G_1)x^6y^6. \\
&= |E_{(2,4)}|x^2y^4 + |E_{(2,5)}|x^2y^5 + |E_{(3,5)}|x^3y^5 + |E_{(3,6)}|x^3y^6 + |E_{(4,4)}|x^4y^4 + |E_{(4,5)}|x^4y^5 \\
&+ |E_{(5,5)}|x^5y^5 + |E_{(5,6)}|x^5y^6 + |E_{(6,6)}|x^6y^6
\end{aligned}
$$

Now, using these, we have,

$$
\begin{aligned}
D_x\big|_{x=y=1} &= 8q^2(q-2)+2(7p-26q)+pq(6pq-18p+7q+25)+4(3p^2-4q^2)+104. \\
D_y\big|_{x=y=1} &= pq(6pq+5q+131)+12(p^2+q^2)-2(20p+41q). \\
S_x\big|_{x=y=1} &= pq[\frac{1}{2}p+\frac{4}{15}q-\frac{1}{6}pq+\frac{8}{3}]-\frac{2}{15}q^3-\frac{p}{15}(5p-27)-\frac{q}{60}(159q-313)-\frac{68}{15}. \\
S_y\big|_{x=y=1} &= pq\left[\frac{1}{2}p+\frac{7}{10}q-\frac{1}{6}pq+\frac{1}{3}\right]-\frac{p}{15}(5p-28)-\frac{q}{60}(119q-295)-\frac{173}{30}.
\end{aligned}
$$

with these cardinalities substituting in topological indices definitions we get required results.

Figure 7 shows the graph of the M-polynomial of the 2D-lattice:

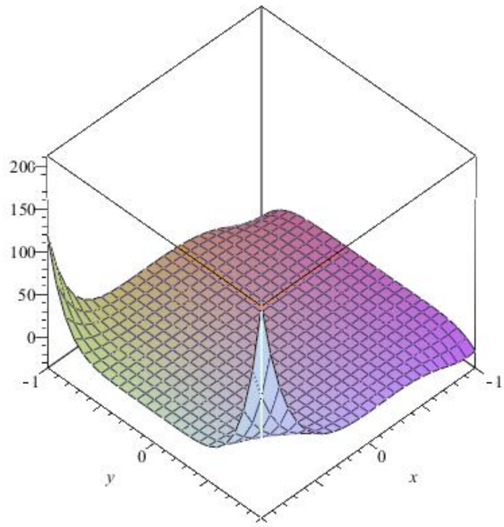

Figure 7: The M-polynomial of semi-total line graph of 2D-lattice

Theorem 3.2. Let H_1 be the semi-total line graph of the nanotube of *$TUC_4C_8(p, q)$* then,

1) $M(H_1,x,y)=4px^2y^5+2qx^3y^3+[2pq(5-q)-4(2p-1)]x^3y^5$
$+[(q-1)(16p-pq+q-2)]x^3y^6+[4p+p(q-1)(q-4)]x^5y^5$
$+[4(p-1)-2p(q-1)(q-4)]x^5y^6+[(q-1)(8p+5q+q(p-q))-10]x^6y^6.$

2) $M_1(H_1)=pq(329+26q)-3q^2(4q-1)-(188p+147q)+78.$

3) $M_2(H_1)=[pq(100+43q)-q^2(6q+39)-5(8p+9q)+10]$
$\times[pq(229-17q)-6q^2(q-7)-2(74p+51q)+68].$

4) $${}^{m}M_2(H_1)=\left[\frac{1}{2}pq\left(\frac{29}{3}-q\right)-\frac{1}{30}(12p+25q)-\frac{1}{30}q^2(5q-24)+\frac{7}{5}\right]$$
$$\times\left[2pq\left(3-\frac{1}{5}q\right)-\frac{1}{3}(10p+7q)-\frac{1}{6}q^2(q+7)+\frac{32}{15}\right].$$

5) $R_\alpha(H_1)=[pq(100+43q)-q^2(6q+39)-5(8p+9)+10]^\alpha$
$\times[pq(229-17q)-6q^2(q-7)-2(74p+51q)+68]^\alpha.$

6) $$R'_\alpha(H_1)=\left[\frac{1}{2}pq(\frac{29}{3}-q)-\frac{1}{30}(12p+25q)-\frac{1}{30}q^2(5q-24)+\frac{7}{5}\right]^\alpha$$
$$\times\left[2pq(3-\frac{1}{5}q)-\frac{1}{3}(10p+7q)-\frac{1}{6}q^2(q+7)+\frac{32}{15}\right]^\alpha.$$

7) $SDD(H_1)=[pq(43q+100)-q^2(6q+39)-5(8p+9q)+10]$
$$\times[2pq(3-\frac{1}{5}q)-\frac{1}{3}(10p+7q)-\frac{1}{6}q^2(q+7)+\frac{32}{15}]+[pq(229-17q)$$
$$-6q^2(q-7)-2(74p+51q)+68]\times[\frac{1}{2}pq(\frac{29}{3}-q)-\frac{1}{30}(12p+25q)$$
$$-\frac{1}{30}q^2(5q-24)+\frac{7}{5}].$$

Proof. Let H_1 be the semi-total line graph of the nanotube *$TUC_4C_8[p,q]$*. This graph has $(10pq-p+3q)$ number of vertices and $[q(q-5)-pq(q+4)(q-7)-18p+6]$ number of edges, respectively.

$E_{(2,5)}=\{e=uv\in E(H_1)|d_u=2,d_v=5\}\rightarrow|E_{(2,5)}|=4p$

$E_{(3,3)}=\{e=uv\in E(H_1)|d_u=3,d_v=3\}\rightarrow|E_{(3,3)}|=2q$

$E_{(3,5)}=\{e=uv\in E(H_1)|d_u=3,d_v=5\}\rightarrow|E_{(3,5)}|=2pq(5-q)-4(2p-1)$

$E_{(3,6)}=\{e=uv\in E(H_1)|d_u=3,d_v=6\}\rightarrow|E_{(3,6)}|=(q-1)(16p-q(p+1)-2)$

$E_{(5,5)}=\{e=uv\in E(H_1)|d_u=5,d_v=5\}\rightarrow|E_{(5,5)}|=4p+p(q-1)(q-4)$

$E_{(5,6)}=\{e=uv\in E(H_1)|d_u=5,d_v=6\}\rightarrow|E_{(5,6)}|=4(p-1)-2p(q-1)(q-4)$

$E_{(6,6)}=\{e=uv\in E(H_1)|d_u=6,d_v=6\}\rightarrow|E_{(6,6)}|=(q-1)[8p+5q+q(p-q)-10].$

Thus,

$$
\begin{aligned}
M(H_1,x,y) &= \sum_{i\le j} m_{ij}(H_1)x^i y^j \\
&= \sum_{2\le 5} m_{25}(H_1)x^2y^5 + \sum_{i=j=3} m_{33}(H_1)x^3y^3 + \sum_{3\le 5} m_{35}(H_1)x^3y^5 + \sum_{3\le 6} m_{36}(H_1)x^3y^6 \\
&+ \sum_{i=j=5} m_{55}(H_1)x^5y^5 + \sum_{5\le 6} m_{56}(H_1)x^5y^6 + \sum_{i=j=6} m_{66}(H_1)x^6y^6. \\
&= \sum_{uv\in E_{(2,5)}} m_{25}(H_1)x^2y^5 + \sum_{uv\in E_{(3,3)}} m_{33}(H_1)x^3y^3 + \sum_{uv\in E_{(3,5)}} m_{35}(H_1)x^3y^5 + \sum_{uv\in E_{(3,6)}} m_{36}(H_1)x^3y^6 \\
&+ \sum_{uv\in E_{(5,5)}} m_{55}(H_1)x^5y^5 + \sum_{uv\in E_{(5,6)}} m_{56}(H_1)x^5y^6 + \sum_{uv\in E_{(6,6)}} m_{66}(H_1)x^6y^6. \\
&= |E_{(2,5)}|x^2y^5 + |E_{(3,3)}|x^3y^3 + |E_{(3,5)}|x^3y^5 + |E_{(3,6)}|x^3y^6 + |E_{(5,5)}|x^5y^5 \\
&+ |E_{(5,6)}|x^5y^6 + |E_{(6,6)}|x^6y^6
\end{aligned}
$$

Since by above expression we obtain

$$
\begin{aligned}
D_x\big|_{x=y=1} &= pq(43q+100) - q^2(6q+39) - 4(8p+9q) + 10. \\
D_y\big|_{x=y=1} &= pq(229-17q) - 6q^2(q-7) - 2(74p+51q) + 68. \\
S_x\big|_{x=y=1} &= \frac{1}{2}pq(\frac{29}{3}-q) - \frac{1}{30}(12p+25q) - \frac{1}{30}q^2(5q-24) + \frac{7}{5}. \\
S_y\big|_{x=y=1} &= 2pq(3-\frac{1}{5}q) - \frac{1}{3}(10p+7q) - \frac{1}{6}q^2(q+7) + \frac{32}{15}.
\end{aligned}
$$

with these cardinalities substituting in topological indices definitions we get required results. Below figure 8 shows the graph of the M-polynomial of the nanotube:

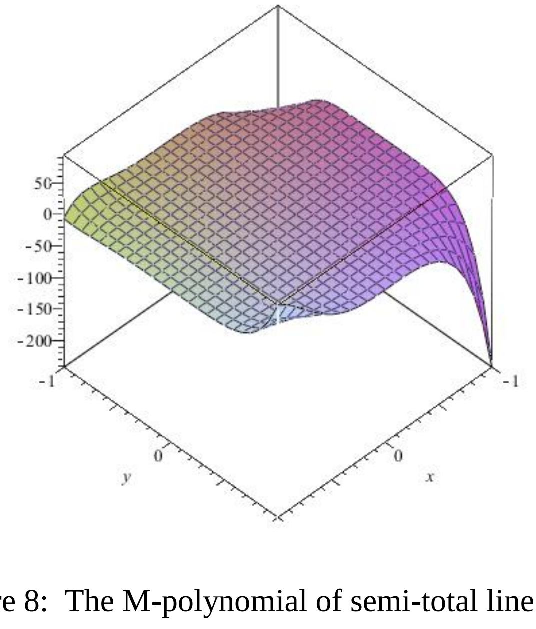

Figure 8: The M-polynomial of semi-total line graph of nanotube

Theorem 3.3. Let K_1 be the semi-total line graph of the nanotorus of *TUC₄C₈[p,q]*. Then,

1) $M(K_1,x,y)=2(p+q)x^3y^3+2(p+q+6pq)x^3y^6+4(3pq-p-q)x^6y^6.$

2) $M_1(K_1)=18(14pq-p-q).$

3) $M_2(K_1)=72(9pq-p-q)(24pq-p-q).$

4) ${}^{m}M_2(K_1)=\{\frac{2}{9}(3pq+p+q)(9pq+p+q).$

5) $R_\alpha(K_1)=[72(9pq-p-q)(24pq-p-q)]^\alpha.$

6) $R'_\alpha(K_1)=\left(\frac{2}{9}(3pq+p+q)(9pq+p+q)\right)^\alpha.$

7) $SDD(K_1)=8(9pq+p+q)(11pq-p-q).$

Proof. Let $k_1$be the semi-total line graph of the nanotorus of *TUC₄C₈[p,q]*. This graph has $(10pq+3(p+q))$ number of vertices and $24pq$ number of edges respectively.

$E_{(3,3)}=\{e=uv\in E(K_1)|d_u=3,d_v=3\}\to|E_{(3,3)}|=2(p+q).$

$E_{(3,6)}=\{e=uv\in E(K_1)|d_u=3,d_v=6\}\to|E_{(3,6)}|=2(p+q+6pq).$

$E_{(6,6)}=\{e=uv\in E(K_1)|d_u=6,d_v=6\}\to|E_{(6,6)}|=4(3pq-p-q).$

Thus,

$$M(K_1,x,y)=\sum_{i\le j}m_{ij}(K_1)x^iy^j$$
$$=\sum_{i=j=3}m_{33}(K_1)x^3y^3++\sum_{3\le 6}m_{36}(K_1)x^3y^6+\sum_{i=j=6}m_{66}(K_1)x^6y^6.$$
$$=\sum_{uv\in E_{(3,3)}}m_{33}(K_1)x^3y^3+\sum_{uv\in E_{(3,6)}}m_{36}(K_1)x^3y^6+\sum_{uv\in E_{(6,6)}}m_{66}(K_1)x^6y^6.$$
$$=|E_{(3,3)}|x^3y^3+|E_{(3,6)}|x^3y^6+|E_{(6,6)}|x^6y^6.$$

Now, using this above equation, we have,

$$D_x|_{x=y=1}=12(9pq-p-q).$$
$$D_y|_{x=y=1}=6(24pq-p-q).$$
$$S_x|_{x=y=1}=6pq+\frac{2}{3}(p+q).$$
$$S_y|_{x=y=1}=3pq+\frac{1}{3}(p+q).$$

with these cardinalities substituting in topological indices definitions we get required results.

Figure 9 shows the graph of the *M*-polynomial of the nanotorus of the semi-total line graph:

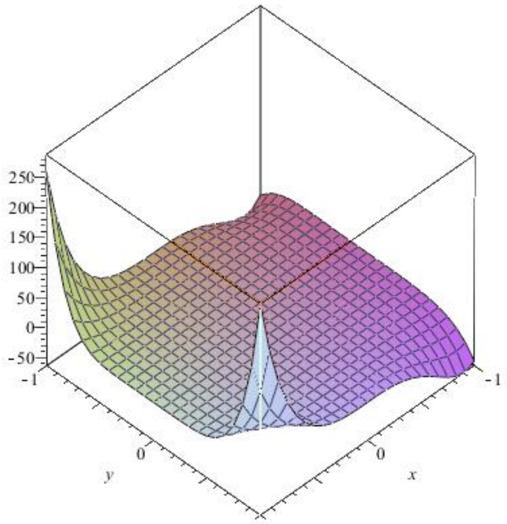

Figure 9: M-polynomial of the nanotorus of semi-total line graph

4. Semi-total point graph of $TUC_4C_8[p,q]$

In this section, we compute the closed forms of the M -polynomials of the semi-total point graph of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$ and the structure of the graph depicted in Figure 10.

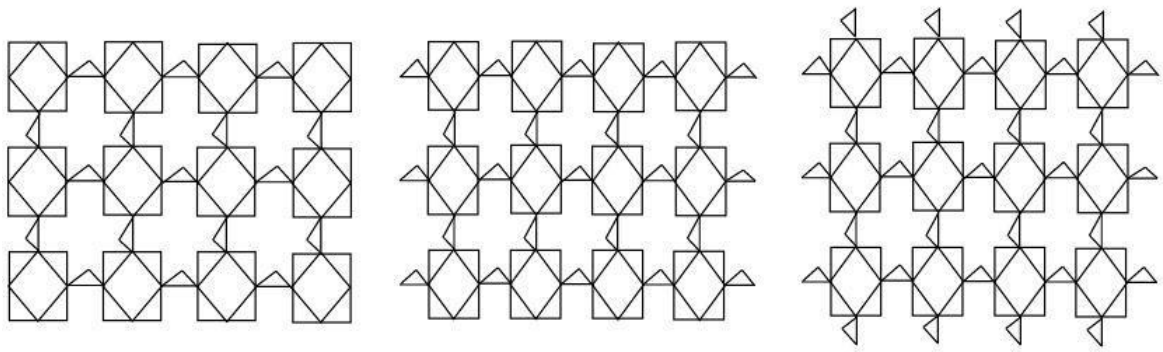

Figure 10: The 2D-lattice, nanotube and nanotorus of semi-total point graph

Theorem 4.1. Let G_2 be the semi-total point graph of the 2D-lattice of $TUC_4C_8(p,q)$. Then

1) $M(G_2, x.y) = 4(p+q)x^2y^4 + [6(p-q) - 2pq(q-1)(q-5)]x^2y^6 + 4x^4y^4 + 4(p+q-2)x^4y^6 + [6pq - 5(p+q) + 4]x^6y^6.$

2) $M_1(G_2) = 4(13p - 11q) - 8pq(2q^2 - 6q + 5)$

3) $M_2(G_1) = [6(p-3q) - 4pq(q^2 + 6q + 4) + 8] \times [2(23p - 13q) - 12pq(q^2 - 6q + 2) - 8].$

4) $^{m}M_2(G_1)=\frac{1}{36}[(31p-5q)-6pq(q^2+6q+4)+8]\times[(11p-q)$
$-12pq(q^2-6q+2)+2].$

5) $R_\alpha(G_1)=[6(p-3q)-4pq(q^2+6q+4)+8]^\alpha\times[2(23p-13q)$
$-12pq(q^2-6q+2)-8]^\alpha$

6) $R_\alpha^{'}(G_1)=\left(\frac{1}{36}\right)^\alpha[(31p-5q)-6pq(q^2-6q+4)-2]^\alpha$
$\times[(11p-q)-2pq(q^2-6q+2)+2]^\alpha$

7) $SDD(G_1)=\left[(p-3q)-\frac{2}{3}pq(q^2+6q+4)+\frac{4}{3}\right]\times[(11p-q)-2pq(q^2-6q+2)+2]$
$+\left[\frac{1}{3}(23p-13q)-12pq(q^2-6q+2)-\frac{4}{3}\right]\times[(31p-5q)-6pq(q^2-6q+4)-2].$

Proof. Let G_2 be the semi-total point graph of the nanotube of $TUC_4C_8(p,q)$. The graph has $(10pq-p-q)$ number of vertices and $(3(3p-q)-2pq(q^2-6q+2))$ number of edges respectively. From figure there are five types of edge partitions:

$$E_{(2,4)}=\{e=uv\in E(G_2)|d_u=2,d_v=4\}\rightarrow|E_{(2,4)}|=4(p+q)$$
$$E_{(2,6)}=\{e=uv\in E(G_2)|d_u=2,d_v=6\}\rightarrow|E_{(2,6)}|=[6(p-q)-2pq(q-1)(q-5)]$$
$$E_{(4,4)}=\{e=uv\in E(G_2)|d_u=4,d_v=4\}\rightarrow|E_{(4,4)}|=4$$
$$E_{(4,6)}=\{e=uv\in E(G_2)|d_u=4,d_v=6\}\rightarrow|E_{(4,6)}|=4(p+q-2)$$
$$E_{(6,6)}=\{e=uv\in E(G_2)|d_u=6,d_v=6\}\rightarrow|E_{(6,6)}|=[6pq-5(p+q)+4]$$

Thus,

$$M(G_2,x,y)=\sum_{i\le j}m_{ij}(G_2)x^iy^j$$
$$=\sum_{2\le 4}m_{24}(G_2)x^2y^4+\sum_{2\le 6}m_{26}(G_2)x^2y^6+\sum_{i=j=4}m_{44}(G_2)x^4y^5$$
$$+\sum_{4\le 6}m_{46}(G_2)x^4y^6+\sum_{i=j=6}m_{66}(G_2)x^6y^6.$$
$$=\sum_{uv\in E_{(2,4)}}m_{24}(G_2)x^2y^4+\sum_{uv\in E_{(2,6)}}m_{26}(G_2)x^2y^6+\sum_{uv\in E_{(4,4)}}m_{44}(G_2)x^4y^4$$
$$+\sum_{uv\in E_{(4,6)}}m_{46}(G_2)x^4y^6+\sum_{uv\in E_{(6,6)}}m_{66}(G_2)x^6y^6.$$

$$=|E_{(2,4)}|x^2y^4+|E_{(2,6)}|x^2y^6+|E_{(4,4)}|x^4y^4+|E_{(4,6)}|x^4y^6+|E_{(6,6)}|x^6y^6.$$

Here, we have,

$$D_x\big|_{x=y=1} = 6(p-3q) - 4pq(q^2+6q+4) + 8$$

$$D_y\big|_{x=y=1} = 2(23p-13q) - 12pq(q^2-6q+2) - 8$$

$$S_x\big|_{x=y=1} = \frac{1}{6}(31p-5q) - pq(q^2-6q+4) - \frac{1}{3}$$

$$S_y\big|_{x=y=1} = \frac{1}{6}(11p-q) - \frac{1}{3}pq(q^2-6q+2) + \frac{1}{3}$$

with these substituting in topological indices definitions we get required results.

Figure 11 shows the graph of the M-polynomial of the 2D-lattice:

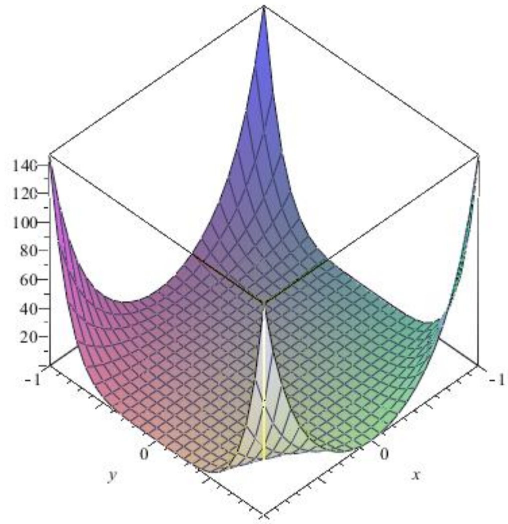

Figure 11: The M-polynomial of semi-total point graph of 2D-lattice

Theorem 4.2. Let H_2 be the semi-total point graph of nanotube of $TUC_4C_8(p,q)$ then,

1) $M(H_2,x,y) = 4px^2y^4 + [6p(2q-1)+2q]x^2y^6 + 4px^4y^6 + (6pq-5p+q)x^6y^6$

2) $M_1(H_2) = 28(6p+1) - 44p.$

3) $M_2(H_2) = 4[5q(6p+1)-9p][9q(6p+1)-13p].$

4) ${}^mM_2(H_2) = \left[7pq - \frac{1}{6}(5p-37q)\right]\left[3pq - \frac{1}{6}(p-3q)\right].$

5) $R_\alpha(H_2) = [4(5q(6p+1)-9p)(9q(6p+1)-13p)]^\alpha.$

6) $R'_\alpha(H_2) = \left[\left(7pq - \frac{1}{6}(5p-37q)\right)\left(3pq - \frac{1}{6}(p-3q)\right)\right]^\alpha.$

7) $SDD(H_2) = [10p(6p+1)-18p] \times \left[3pq - \frac{1}{6}(p-3q)\right] + [18q(6p+1)-26p]$
$\times \left[7pq - \frac{1}{6}(5p-37q)\right].$

Proof. Let H_2 be the semi-total point graph of nanotube $TUC_4C_8(p,q)$. The graph has $(10pq - p + 3q)$ number of vertices and $(18pq - 3(p-q))$ number of edges respectively.

$$E_{(2,4)} = \{e = uv \in E(H_2) | d_u = 2, d_v = 4\} \to |E_{(2,4)}| = 4p$$

$$E_{(2,6)} = \{e = uv \in E(H_2) | d_u = 2, d_v = 6\} \to |E_{(2,6)}| = [6p(2q-1) + 2q]$$

$$E_{(4,6)} = \{e = uv \in E(H_2) | d_u = 4, d_v = 6\} \to |E_{(4,6)}| = 4p$$

$$E_{(6,6)} = \{e = uv \in E(H_2) | d_u = 6, d_v = 6\} \to |E_{(6,6)}| = (6pq - 5p + q)$$

Thus,

$$M(H_2, x, y) = \sum_{i \le j} m_{ij}(H_2) x^i y^j$$

$$= \sum_{2 \le 4} m_{24}(H_2) x^2 y^4 + \sum_{2 \le 6} m_{26}(H_2) x^2 y^6 + \sum_{4 \le 6} m_{44}(H_2) x^4 y^6 + \sum_{i=j=6} m_{66}(G_2) x^6 y^6.$$

$$= |E_{(2,4)}| x^2 y^4 + |E_{(2,6)}| x^2 y^6 + |E_{(4,6)}| x^4 y^6 + |E_{(6,6)}| x^6 y^6.$$

Now,

$$D_x\big|_{x=y=1} = 10q(6p+1) - 18p$$

$$D_y\big|_{x=y=1} = 18q(6p+1) - 26p.$$

$$S_x\big|_{x=y=1} = 7pq - \frac{1}{6}(5p - 37q).$$

$$S_y\big|_{x=y=1} = 3pq - \frac{1}{6}(p - 3q).$$

with these substituting in topological indices definitions we get required results.

From the figure 12 shows the graph of nanotube of M-polynomial:

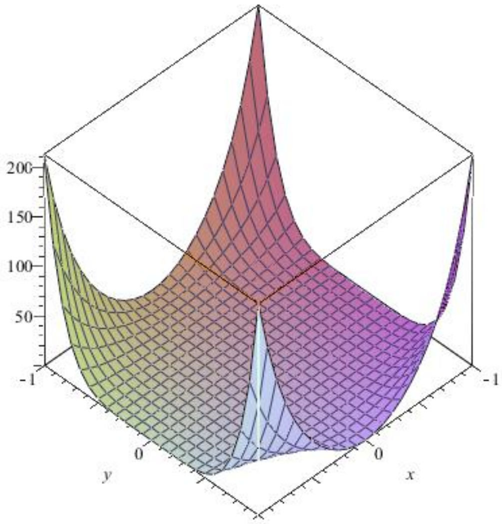

Figure 12: The M-polynomial of semi-total point graph of nanotube

Theorem 4.3. Let K_2 be the semi-total point graph of nanotorus of $TUC_4C_8(p,q)$ then,

1) $M(K_2, x, y) = 2(p+q+6pq)x^2y^6 + (6pq+p+q)x^6y^6$

2) $M_1(K_2) = 28(6pq+p+q).$

3) $M_2(H_2) = 180(6pq+p+q)^2.$

4) ${}^mM_2(K_2) = \frac{7}{12}(6pq+p+q)^2.$

5) $R_\alpha(K_2) = [180(6pq+p+q)]^{2\alpha}.$

6) $R'_\alpha(K_2) = \left[\frac{7}{12}(6pq+p+q)^2\right]^\alpha.$

7) $SDD(H_2) = 26(6pq+p+q)^2.$

Proof. Let K_2 be the semi-total point graph of nanotorus $TUC_4C_8(p,q)$. The graph has $(10pq - 3(p+q))$ number of vertices and $3(6pq+p+q)$ number of edges respectively.

$E_{(2,6)} = \{e = uv \in E(K_2) | d_u = 2, d_v = 6\} \rightarrow |E_{(2,6)}| = 2(p+q+6pq)$

$E_{(6,6)} = \{e = uv \in E(K_2) | d_u = 6, d_v = 6\} \rightarrow |E_{(6,6)}| = (6pq+p+q)$

Thus,

$$M(K_2, x, y) = \sum_{i \le j} m_{ij}(K_2)x^i y^j$$

$$= \sum_{2 \le 6} m_{26}(K_2)x^2y^6 + \sum_{i=j=6} m_{66}(K_2)x^6y^6.$$

$$= |E_{(2,6)}|x^2y^6 + |E_{(6,6)}|x^6y^6.$$

Now,

$$D_x|_{x=y=1} = 10(6pq+p+q)$$

$$D_y|_{x=y=1} = 18(6pq+p+q)$$

$$S_x|_{x=y=1} = \frac{7}{6}(6pq+p+q)$$

$$S_y|_{x=y=1} = \frac{1}{2}(6pq+p+q)$$

with these substituting in topological indices definitions we get required results.

From the figure 13 shows the graph of nanotorus of M-polynomial:

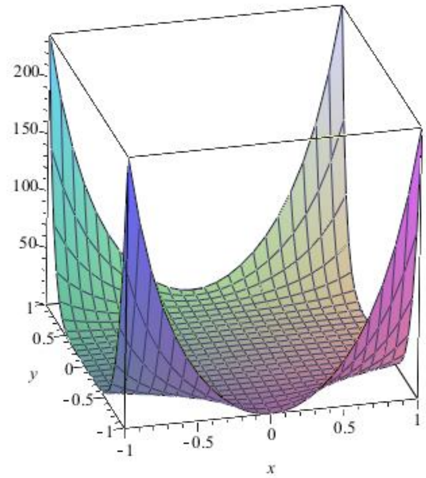

Figure 13: The M-polynomial of semi-total point graph of nanotorus

CONCLUSIONS

In this article, we computed the closed form of the M-polynomial for the 2*D*-lattices, nanotubes and nanotorus. We derived certain degree-based topological indices for these nanostructures. We also plot some surfaces associated with these nanostructures that show the dependence of each topological index on the parameters of the structure. These indices can help us to understand its physical features, chemical and biological activities such as the boiling point, the heat of formation, the fracture toughness, the strength, the conductivity and the hardness. From this point of view, a topological index can be regarded as a score function that maps each molecular structure to a real number and is used as a descriptor of the molecule under testing.

ACKNOWLEDGEMENTS

First and second authors were supported by the research fund of Department of Science and Technology, project no: SR/WOS-A/PM-43/2016. Third author was supported by the research fund of Uludag University project no F-2015/17.

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