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Topological Properties of Networks Using M-Polynomial Approach

Sourav Mondal 1 , Nilanjan De $^{2^\ast}$ and Anita Pal 1

¹*Department of mathematics, NIT Durgapur, India.*

²*Department of Basic Sciences and Humanities (Mathematics), Calcutta Institute of Engineering and Management, Kolkata, India.* **Corresponding author*

Abstract

The M-polynomial is one of the algebraic polynomials, that is useful in theoretical chemistry. It plays significant role in computing the exact expressions of many degree based topological indices. In this report, the M-polynomial of the benzene ring embedded in P-type-surface in 2D network and the Tickysim SpiNNaker Model (TSM) sheet are derived. Using those M-polynomials, some degree based topological indices are derived. In addition, the results are interpreted graphically.

Keywords: M-polynomial, Degree based topological index, benzene ring embedded in P-type-surface in 2D network, Tickysim SpiNNaker Model (TSM) sheet. 2010 Mathematics Subject Classification: Primary: 05C35; Secondary: 05C07, 05C40.

1. Introduction

Throughout this article we consider simple connected graph. Let *V*(*G*) and *E*(*G*) be vertex set and edge set of a graph *G*, respectively. The total number of edges incident to $v \in V(G)$ is known as the degree of *v* and is denoted by d_v . Mathematical models play an important role in the analysis of important concepts of chemistry. Topological index plays key role in such modeling. Topological index is a mapping from the collection of all graphs to the set of real numbers that yields same value for isomorphic graphs. These numerical quantities corresponding to a graph are effective in correlating the structure with different physico-chemical properties, chemical reactivity, and biological activities. These indices are evaluated by formal definitions. Instead of calculating different topological indices of a specific category [\[1,](#page-8-0) [2\]](#page-8-1), we can use a compact general method related to polynomial for calculating the same. For instance, in the domain of distance-based topological indices Wiener polynomial is a general polynomial whose derivatives at 1 yield Weiner and Hyper Weiner indices [\[2\]](#page-8-1). There are many such polynomials such as PI polynomial [\[3\]](#page-8-2), Theta polynomial [\[4\]](#page-8-3) etc.

In the area of degree-based topological indices, M-polynomial [\[1\]](#page-8-0) perform similar role to compute closed expressions of many degree based topological indices [\[1,](#page-8-0) [5\]](#page-8-4). Thus computation of degree based topological indices reduce to evaluation of a single polynomial. Moreover, detailed analysis of this polynomial can yield new insights in the knowledge of degree based topological indices.

About a quarter of a century OKeeffe et al. [[16\]](#page-8-5) distributed a letter managing two 3D systems of benzene one of the structure (figure [3.1\)](#page-2-0) called 6.82P (additionally polybenzene) and has a space gathering place Im3m, compared to the P-type surface. This actually inserts the hexagon-fix into the negative ebb and flow P surface. The P-type surface in the Euclidean space is coordinated with the Cartesian arrangements. The peruser can find out more about this intermittent surface in [\[17,](#page-8-6) [18\]](#page-8-7). This structure had to be combined as 3D carbon solids. This goal was to awaken researchers' enthusiasm for the atomic recognition in carbon nanoscience of such pleasant thoughts. The graph of the benzene ring embedded in P-type-surface network, shown in figure [3.1,](#page-2-0) contains 24*mn* nodes and 32*mn*−2*m*−2*n* edges.

Inter-chip architectures are considered as graphs in which nodes are supposed to be devices and the edges to be the topology used between devices. Hexagonal torus (12×12) is one of the network topologies utilized in this model. Each vertex is associated to six incident nodes in this topology. We also consider the finite TSM sheet which is obtained by hexagonal torus. For more discussion, see [\[19\]](#page-8-8). The graph of the Tickysim SpiNNaker Model (TSM) sheet, shown in figure [3.2,](#page-4-0) has *mn* nodes and 3*mn*−2*m*−2*n*+1 edges.

A. Ahmed [\[20\]](#page-8-9) discussed the topological properties of benzene ring embedded in P-type-surface network. In [\[21\]](#page-8-10), topological properties of the Tickysim SpiNNaker Model are studied. Kwun et al [\[22\]](#page-8-11) derived some degree based topological indices of V-Phenylenic Nanotubes and Nanotori using M-polynomial approach. Present authors [\[23\]](#page-8-12) did the same work for line graph of subdivision graph of some composite graphs. For more works related to this topic, readers are referred to [\[24,](#page-8-13) [25,](#page-8-14) [26,](#page-8-15) [27\]](#page-8-16). The goal of this article is to compute some degree based topological indices of the benzene ring embedded in P-type-surface network and Tickysim SpiNNaker Model (TSM) sheet using M-polynomial.

Email addresses: souravmath94@gmail.com (Sourav Mondal), de.nilanjan@rediffmail.com (Nilanjan De), anita.buie@gmail.com (Anita Pal)

2. Basic definitions and literature review

Definition 2.1. *The M-polynomial of a graph G is defined as,*

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

Where $m_{ij}(G)$ is the total count of edges $uv \in E(G)$ such that $\{d_u, d_v\} = \{i, j\}$. We use $M(G)$ for $M(G; x, y)$ in this article.

Any degree based topological indices for a graph *G* can be expressed as,

$$
I(G) = \sum_{uv \in E(G)} f(d_u, d_v),
$$

where $f = f(x, y)$ is a function appropriately selected for possible chemical applications [\[6\]](#page-8-17). The above result can also be written as

$$
I(G) = \sum_{i \leq j} m_{ij}(G) f(i, j).
$$

Gutman and Trinajstic introduced Zagreb indices [[7\]](#page-8-18). The first Zagreb index is defined as,

$$
M_1(G) = \sum_{v \in V(G)} (d_v)^2
$$

The second Zagreb index is defined as,

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

The forgotten topological index is defined as,

$$
F(G) = \sum_{uv \in E(G)} [d_u^2 + d_v^2].
$$

The second modified Zagreb index is defined as,

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

Bollobas and Erdos [\[8\]](#page-8-19) and Amic et al. [\[9\]](#page-8-20) presented the idea of the generalized Randic index and discussed widely in both chemistry and mathematics [\[10\]](#page-8-21). For more discussion, readers are referred [\[11,](#page-8-22) [12\]](#page-8-23). The general Randić index is defined as,

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

The inverse Randić index is defined as,

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

The Symmetric division index of a connected graph *G*, is defined as,

$$
SDD(G) = \sum_{uv \in E(G)} \left\{ \frac{min(d_u, d_v)}{max(d_u, d_v)} + \frac{max(d_u, d_v)}{min(d_u, d_v)} \right\}.
$$

The Harmonic index [\[13\]](#page-8-24) is defined as,

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

The inverse sum indeg index $[14]$ is given by

$$
I(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v}.
$$

The augmented Zagreb index proposed by Furtula et al. [\[15\]](#page-8-26) is defined as,

$$
A(G) = \sum_{uv \in E(G)} \{ \frac{d_u d_v}{d_u + d_v - 2} \}^3.
$$

The relations of some degree-based topological indices with the M-polynomial are shown in the table [1.](#page-2-1)

| Topological Index | f(x,y) | Derivation from $M(G)$ |
|-------------------|--|--|
| M_1 | $x + y$ | $\overline{(D_x + D_y)}(M(G)) _{x=y=1}$ |
| M_2 | xy | $\overline{(D_xD_y)(M(G))} _{x=y=1}$ |
| F | $x^2 + y^2$ | $\frac{1}{(D_x^2 + D_y^2)(M(G)) _{x=y=1}}$ |
| mM_2 | xγ | $\overline{(S_xS_y)(M(G))} _{x=y=1}$ |
| R_{α} | $(xy)^{\overline{\alpha}}$ | $\overline{(D_x^{\alpha}D_y^{\alpha})(M(G)) _{x=y=1}}$ |
| RR_{α} | $(xv)^{\alpha}$ | $\overline{(S^\alpha_x S^\alpha_y)}(M(G)) _{x=y=1}$ |
| SDD | x^2+y^2 | $(D_xS_y + S_xD_y)(M(G)) _{x=y=1}$ |
| H | $\frac{xy}{2}$ $\frac{\overline{x+y}}{\overline{xy}}$ | $2S_xJ(M(G)) _{x=1}$ |
| | $x+y$ | $S_xJD_xD_y(M(G)) _{x=1}$ |
| A | $(x+y-2)^3$ | $\sqrt{S_{x}^{3}Q_{-2}JD_{x}^{3}D_{y}^{3}(M(G))} _{x=1}$ |

Table 1: Derivation of some degree based topological indices

Where,

$$
D_x(f(x,y)) = x \frac{\partial (f(x,y))}{\partial x}, D_y(f(x,y)) = y \frac{\partial (f(x,y))}{\partial y},
$$

$$
S_x(f(x,y)) = \int_0^x \frac{(f(t,y))}{t} dt, S_y(f(x,y)) = \int_0^y \frac{(f(x,t))}{t} dt
$$

$$
J(f(x, y)) = f(x, x), Q_{\alpha}(f(x, y)) = x^{\alpha} f(x, y).
$$

Figure 3.1: Benzene ring embedded in p-type surface in 2D network .

3. Main Results

In this part, we give our main computational results and divide the section in two subsections.

3.1. Computational aspects of Benzene ring embedded in p-type surface in 2D network.

We compute the *M*-polynomial of the benzene ring embedded in p-type surface network in the following theorem.

Theorem 1. *Let G be the benzene ring embedded in p-type surface network. Then we have,*

$$
M(G) = 4(m+n)x^{2}y^{2} + 16mnx^{2}y^{3} + 2(8mn - 3m - 3n)x^{3}y^{3}.
$$

Proof. The edge set of *G* can be partitioned as,

 $|E_{\{2,2\}}| = |\{uv \in E(G) : d_u = 2, d_v = 2\}| = 4(m+n) = m_{22}.$

 $|E_{\{2,3\}}| = |\{uv \in E(G) : d_u = 2, d_v = 3\}| = 16mn = m_{23}.$

$$
|E_{\{3,3\}}| = |\{uv \in E(G) : d_u = 3, d_v = 3\}| = 2(8mn - 3m - 3n) = m_{33}.
$$

From the definition, the *M*-polynomial of *G* is obtained bellow.

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

= $m_{22} x^2 y^2 + m_{23} x^2 y^3 + m_{33} x^3 y^3$
= $4(m+n)x^2 y^2 + 16mnx^2 y^3 + 2(8mn - 3m - 3n)x^3 y^3$.

This completes the proof.

Now using this *M*-polynomial, we calculate some degree based topological indices of the benzene ring embedded in p-type surface network in the following theorem.

Theorem 2. *Let G be the benzene ring embedded in p-type surface network. Then we have,*

1. $M_1(G) = 4(44mn - 5m - 5n)$, 2. $M_2(G) = 2(120mn - 19m - 19n)$ *3. F*(*G*) = 4(124*mn*−19*m*−19*n*)*,* 4. $M_2^m(G) = \frac{1}{3}(\frac{40}{3}mn+m+n)$, 5. $R_{\alpha}(G) = 2^{2(\alpha+1)}(m+n) + 2^{(4+\alpha)}3^{\alpha}mn + 2.3^{2\alpha}(8mn-3m-3n)$, 6. $RR_{\alpha}(G) = 2^{(1-\alpha)}(m+n) + 2^{(4-\alpha)}3^{-\alpha}mn + 2.3^{-2\alpha}(8mn-3m-3n)$, *7.* $SDD(G) = \frac{200}{3}mn - 4m - 4n$, *8.* $H(G) = \frac{176}{15}$ *mn*, 9. $I(G) = \frac{216}{5}mn - 5m - 5n$, *10.* $A(G) = \frac{1241}{4}mn - \frac{1163}{32}m - \frac{1163}{32}n$.

Proof. Let $M(G) = f(x, y) = 4(m+n)x^2y^2 + 16mnx^2y^3 + 2(8mn-3m-3n)x^3y^3$. Then we have,

$$
(D_x + D_y)(f(x, y)) = 16(m+n)x^2y^2 + 80mnx^2y^3 + 12(8mn - 3m - 3n)x^3y^3,
$$

\n
$$
D_x D_y(f(x, y)) = 16(m+n)x^2y^2 + 96mnx^2y^3 + 18(8mn - 3m - 3n)x^3y^3,
$$

\n
$$
(D_x^2 + D_y^2)(f(x, y)) = 32(m+n)x^2y^2 + 208mnx^2y^3 + 36(8mn - 3m - 3n)x^3y^3,
$$

\n
$$
S_x S_y(f(x, y)) = (m+n)x^2y^2 + \frac{8}{3}mnx^2y^3 + \frac{2}{9}(8mn - 3m - 3n)x^3y^3,
$$

\n
$$
D_x^{\alpha} D_y^{\alpha}(f(x, y)) = 2^{2(\alpha+1)}(m+n)x^2y^2 + 2^{4+\alpha}3^{\alpha}mnx^2y^3 + 2(3^{2\alpha})(8mn - 3m - 3n)x^3y^3,
$$

\n
$$
S_x^{\alpha} S_y^{\alpha}(f(x, y)) = 2^{2(1-\alpha)}(m+n)x^2y^2 + 2^{4-\alpha}3^{-\alpha}mnx^2y^3 + 2(3^{-2\alpha})(8mn - 3m - 3n)x^3y^3,
$$

\n
$$
(D_x S_y + S_x D_y)(f(x, y)) = 8(m+n)x^2y^2 + \frac{104}{3}mnx^2y^3 + 4(8mn - 3m - 3n)x^3y^3,
$$

\n
$$
S_x J(f(x, y)) = (m+n)x^4 + \frac{16}{5}mnx^5 + \frac{1}{3}(8mn - 3m - 3n)x^6,
$$

\n
$$
S_x J D_x D_y(f(x, y)) = 4(m+n)x^4 + \frac{96}{5}mnx^5 + 3(8mn - 3m - 3n)x^6,
$$

\n
$$
S_x^3 Q_{-2} J D_x^3 D_y^3(f(x, y)) = 32(m+n)x^2 + 128mnx^3 + \frac{729}{32}(8mn - 3m - 3n)x^4.
$$

Using table 1, we can easily obtain the required result.

3.2. Computational aspects of the Tickysim SpiNNaker Model (TSM) sheet.

We compute the *M*-polynomial of the TSM sheet in the following theorem.

Theorem 3. *Let G be the TSM sheet. Then we have,*

$$
M(G) = 4x^2y^4 + 4x^3y^4 + 2x^3y^6 + 2(m+n-5)x^4y^4 + 4(m+n-5)x^4y^6 + (3mn-8m-8n+21)x^6y^6.
$$

Proof. The edge set of *G* has partitions as follows,

$$
|E_{\{2,4\}}| = |\{uv \in E(L(S(T_{n,k}))) : d_u = 2, d_v = 4\}| = 4 = m_{24}.
$$

$$
|E_{\{3,4\}}| = |\{uv \in E(L(S(T_{n,k}))) : d_u = 3, d_v = 4\}| = 4 = m_{34}.
$$

$$
|E_{\{3,6\}}| = |\{uv \in E(L(S(T_{n,k}))) : d_u = 3, d_v = 6\}| = 2 = m_{36}.
$$

$$
|E_{\{4,4\}}| = |\{uv \in E(L(S(T_{n,k}))) : d_u = 4, d_v = 4\}| = 2(m+n-5) = m_{44}.
$$

$$
|E_{\{4,6\}}| = |\{uv \in E(L(S(T_{n,k}))) : d_u = 4, d_v = 6\}| = 4(m+n-5) = m_{46}.
$$

 \Box

 \Box

Figure 3.2: The graphical representation of the TSM sheet .

Figure 3.3: The M-polynomal of (a) the benzene ring embedded in p-type surface network and (b) the TSM sheet.

$$
|E_{\{6,6\}}| = |\{uv \in E(L(S(T_{n,k}))) : d_u = 6, d_v = 6\}| = 3mn - 8m - 8n + 21 = m_{66}.
$$

From the definition, the *M*-polynomial of *G* is obtained bellow,

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

= $m_{24} x^2 y^4 + m_{34} x^3 y^4 + m_{36} x^3 y^6 + m_{44} x^4 y^4 + m_{46} x^4 y^6 + m_{66} x^6 y^6$
= $4x^2 y^4 + 4x^3 y^4 + 2x^3 y^6 + 2(m + n - 5)x^4 y^4 + 4(m + n - 5)x^4 y^6 + (3mn - 8m - 8n + 21)x^6 y^6$.

This completes the proof.

Now using this *M*-polynomial, we calculate some degree based topological index of the TSM sheet in the following theorem.

Theorem 4. *Let G be the TSM sheet. Then we have,*

1. $M_1(G) = 2(38mn-20m-20n+21)$ 2. $M_2(G) = 4(27mn-40m-40n+58)$ *3.* $F(G) = 2(108mn − 152m − 152n + 211)$ 4. $M_2^m(G) = \frac{1}{12}(mn + \frac{5}{6}m + \frac{5}{6}n + \frac{5}{6}),$ 5. $R_{\alpha}(G) = 2^{3\alpha+2} + 3^{\alpha}2^{2(\alpha+1)} + 2^{\alpha+1}3^{2\alpha} + 2^{4\alpha+1}(m+n-5) + 2^{3\alpha+2}3^{\alpha}(m+n-5) + 6^{2\alpha}(3mn-8m-8n+21)$ 6. $RR_{\alpha}(G) = 2^{2-3\alpha} + 2^{2-2\alpha}3^{-\alpha} + 2^{1-\alpha}3^{-2\alpha} + 2^{1-4\alpha}(m+n-5) + 2^{2-3\alpha}3^{-\alpha}(m+n-5) + 6^{-2\alpha}(3mn-8m-8n+21)$ *7.* $SDD(G) = 6mn - \frac{10}{3}m - \frac{10}{3}n + 2$, 8. $H(G) = \frac{1}{2}mn - \frac{1}{30}m - \frac{1}{30}n - \frac{5}{63}$ 9. $I(G) = 9mn - \frac{52}{5}m - \frac{52}{5}n + \frac{235}{21}$ *10.* $A(G) = \frac{139968}{1000}mn - \frac{9683696}{2700}m - \frac{9683696}{2700}n + 371.448$.

 \Box

 \Box

Figure 3.4: The first Zagreb index of (a) the benzene ring embedded in p-type surface network and (b) the TSM sheet.

Figure 3.5: The second Zagreb index of (a) the benzene ring embedded in p-type surface network and (b) the TSM sheet.

Proof. Let $M(G) = f(x, y) = 4x^2y^4 + 4x^3y^4 + 2x^3y^6 + 2(m+n-5)x^4y^4 + 4(m+n-5)x^4y^6 + (3mn-8m-8n+21)x^6y^6$. Then we have,

$$
(D_x + D_y)(f(x, y)) = 24x^2y^4 + 28x^3y^4 + 18x^3y^6 + 16(m+n-5)x^4y^4 + 40(m+n-5)x^4y^6 + 12(3mn-8m-8n+21)x^5y^6,
$$

\n
$$
D_xD_y(f(x, y)) = 32x^2y^4 + 48x^3y^4 + 36x^3y^6 + 32(m+n-5)x^4y^4 + 96(m+n-5)x^4y^6 + 36(3mn-8m-8n+21)x^6y^6,
$$

\n
$$
(D_x^2 + D_y^2)(f(x, y)) = 80x^2y^4 + 100x^3y^4 + 90x^3y^6 + 64(m+n-5)x^4y^4 + 208(m+n-5)x^4y^6 + 72(3mn-8m-8n+21)x^6y^6,
$$

\n
$$
S_xS_y(f(x, y)) = \frac{1}{2}x^2y^4 + \frac{1}{3}x^3y^4 + \frac{1}{9}x^3y^6 + \frac{1}{8}(m+n-5)x^4y^4 + \frac{1}{6}(m+n-5)x^4y^6 + \frac{1}{36}(3mn-8m-8n+21)x^6y^6,
$$

\n
$$
D_x^{\alpha}D_y^{\alpha}(f(x, y)) = 2^{3\alpha+2}x^2y^4 + 3^{\alpha}4^{\alpha+1}x^3y^4 + 2^{\alpha+1}3^{2\alpha}x^3y^6 + 2^{4\alpha+1}(m+n-5)x^4y^6 + \frac{1}{36}(3mn-8m-8n+21)x^6y^6,
$$

\n
$$
S_x^{\alpha}S_y^{\alpha}(f(x, y)) = 2^{2-3\alpha}x^2y^4 + 2^{2-2\alpha}3^{-\alpha}x^3y^4 + 2^{1-\alpha}3^{-2\alpha}x^3y^6 + 2^{1-4\alpha}(m+n-5)x^4y^4 + 2^{2-3\alpha}3^{-\alpha}(m+n-5)x^4y^6
$$

\n
$$
+6^{-2\alpha}(3mn-8m-8n+21)x^6y^6,
$$

\n
$$
(D_xS_y+S_xD_y)(f(x,y)) = 10x^2y^
$$

Using table 1, the required result can be obtained easily.

Figure 3.6: The forgotten topological index of (a) the benzene ring embedded in p-type surface network and (b) the TSM sheet.

Figure 3.7: The modified second Zagreb index of (a) the benzene ring embedded in p-type surface network and (b) the TSM sheet.

Figure 3.8: The symmetric division index of (a) the benzene ring embedded in p-type surface network and (b) the TSM sheet.

Figure 3.9: The harmonic index of (a) the benzene ring embedded in p-type surface network and (b) the TSM sheet.

Figure 3.10: The inverse sum index index of (a) the benzene ring embedded in p-type surface network and (b) the TSM sheet.

Figure 3.11: The augmented Zagreb index of (a) the benzene ring embedded in p-type surface network and (b) the TSM sheet.

4. Conclusion

We obtained many degree based topological indices for benzene ring embedded in P-type-surface network and Tickysim SpiNNaker Model (TSM) sheet. Firstly, we computed M-polynomial of these graphs and later recovered many degree-based topological indices applying it. Further we have shown the results graphically. These results can play an important role to visualize the topology of the aforesaid networks.

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