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ON TOPOLOGICAL POLYNOMIALS OF WEIGHTED GRAPHS

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ABSTRACT. Two edges *e* and *f* of a plane graph *G* are in relation opposite, *e* op *f*, if they are opposite edges of an inner face of *G*.

Relation op enables the partition the edge set of *G* into opposite edge strips ops. On this ground, Diudea defined Omega and Theta polynomial while Ashrafi et al. defined the Sadhana polynomial. In this paper a weighted version of these polynomials was introduced and several relations between them are demonstrated. Some molecular weights are suggested in view of using the derived topological indices in correlational studies.

Key Words: *Omega polynomial, Sadhana polynomial, Topological indices.*

INTRODUCTION

Mathematical chemistry is a branch of theoretical chemistry that studies molecular structures using mathematical methods, not necessarily referring to quantum mechanics. Chemical graph theory is an important tool for studying molecular structures. At the beginning, let us recall some definitions that will be used in this paper.

Let *G* be a simple molecular graph without directed and multiple edges and without loops, the vertex set *V*(*G*) and edge-sets *E*(*G*) of which representing the atoms and covalent bonds of the molecule. Suppose *G* is a connected molecular graph and $x, y \in V(G)$. The distance *d*(*x, y*) between *x* and *y* is defined as the length of a minimum path between x and y. Two edges *e* = *ab* and *f* = *xy* of *G* are called co-distant, "*e co f*", if and only if *d*(*a,x*) = *d*(*b,y*) = *k* and *d*(*a,y*) = *d*(*b,x*) = *k* + 1 or vice versa, for a non-negative

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integer k. It is easy to see that the relation "*co*" is reflexive and symmetric but it is not necessarily transitive. Set $C(e) = \{ f \in E(G) \mid f \ co \ e \}$. If the relation "*co*" is transitive on $C(e)$ then $C(e)$ is called an orthogonal cut of G. The graph G is called a co-graph if and only if the edge set $E(G)$ is a union of disjoint orthogonal cuts. If any two subsequent edges of an edge-cut sequence are topologically parallel within the same face of the covering, such a sequence is called a quasi-orthogonal cut or *opposite edge strips ops s. If G* is a *co*-graph, then $|c_k| = |s_k|$, *and* $S(G) = \{s_1, s_2, ..., s_k\}$ forms a partition of $E(G)$.

Diudea defined the Ω-polynomial of G on *ops* as [1 – 4]:

$$\Omega(x) = \sum_{i=1}^{k} x^{|s_i|}$$

Another polynomial also related to the ops in G, but counting the *non-opposite* edges is the *Sadhana* polynomial, defined by Ashrafi et al. [5] as:

$$Sd(x) = \sum_{i=1}^{k} x^{|E|-|s_i|}$$

The Sadhana index $Sd(G)$ was defined by Khadikar et al [6, 7] as:

$$Sd(G) = \Sigma_{i=1}^{k} | E(G) | - | s_i | .$$

From the definition of Omega polynomial, one can obtain the Sadhana polynomial by replacing $x^{|s_i|}$.with $x^{|E|-|s_i|}$ in the Omega polynomial. Then the Sadhana index will be the first derivative of $Sd(x)$ evaluated at $x = 1$, see for more details [8 - 14].

RESULTS AND DISCUSSION

Let $e=uv$ be an edge of G and v be an arbitrary vertex. Denote by $w_G(e)$ and $w_G(v)$ the weights of edge e and vertex v, respectively. For each strip s of G, the weight of s can be defined as:

$$w_{G,e}(s) = \sum_{e \in s} w_G(e) ,$$

$$w_{G,v}(S) = \sum_{v \in V(G[s])} w_G(v) = \sum_{uv \in s} \left(w_G(u) + w_G(v) \right) .$$

where $G[s]$ is the induced subgraph in G by s. One can see that if G is a co-graph, then

$$w_e(G) = \sum_{e \in E(G)} w_G(e) = \sum_{s \in S} \sum_{e \in s} w_G(e) .$$

By using the concept of weighted graph, we define three new versions of Omega polynomial: the edge weighted-, vertex weighted- and edge-vertex-weighted Omega polynomial. These new polynomials are defined as follows:

$$\Omega_e(G,x) = \sum_{s\in S}\left\lfloor \frac{w_{G,e}(s)}{|s|}\right\rfloor m(G,s)x^{|s|},$$

$$\Omega_v(G,x) = \sum_{s\in S} m(G,s)x^{\left\lfloor \frac{w_{G,v}(s)}{2}\right\rfloor},$$

$$\Omega_{ev}(G,x) = \sum_{s\in S}\left\lfloor \frac{w_{G,e}(s)}{|s|}\right\rfloor m(G,s)x^{\left\lfloor \frac{w_{G,v}(s)}{2}\right\rfloor}.$$

Obviously, if the weight of each edge and vertex is 1, then

$$\Omega_e(G,x) = \Omega_v(G,x) = \Omega_{ev}(G,x) = \Omega(G,x).$$

Analogously, for Theta and Sadhana polynomials we have:

$$\Theta_e(G,x) = \sum_{c\in C} w_{G,e}(c)m(G,c)x^{|c|},$$

$$\Theta_v(G,x) = \sum_{c\in C} m(G,c)\,|c|\,x^{\left\lfloor \frac{w_{G,v}(c)}{2}\right\rfloor},$$

$$\Theta_{ev}(G,x) = \sum_{c\in C} w_{G,e}(c)m(G,c)x^{\left\lfloor \frac{w_{G,v}(c)}{2}\right\rfloor},$$

$$Sd_e(G,x) = \sum_{c\in C} m(G,c)x^{w_e(G)-w_{G,e}(c)},$$

$$Sd_v(G,x) = \sum_{c\in C}\left\lfloor \frac{w_{G,v}(c)}{2|c|}\right\rfloor m(G,c)x^{|E|-|c|},$$

$$Sd_{ev}(G,x) = \sum_{c\in C}\left\lfloor \frac{w_{G,v}(c)}{2|c|}\right\rfloor m(G,c)x^{w_e(G)-w_{G,e}(c)}.$$

One can see again, if the weight of each edge and vertex be 1, then $\Theta_e(G,x) = \Theta_v(G,x) = \Theta_{ev}(G,x) = \Theta(G,x)$ and $Sd_e(G,x) = Sd_v(G,x) = Sd_{ev}(G,x) = Sd(G,x)$, respectively. Note that, in co-graphs, $|c_k|=|s_k|$, and the symbols c/s interchanges.

Let *G* and *H* be two edge weighted graphs. The Cartesian product graph of G and *H* is a graph with vertex set $V(G \times H) = V(G) \times V(H)$ and edge set

$$E(G\times H) = \{((a,\ b),\ (c,d)) : a=c,\ bd\in E(H)\ or\ b=d, ac\in E(G)\}.$$

Then, the weight of an edge ((a, b),(c, d)) is as follows:

If $a = c$, then $w_{G\times H}(((a, b),(c, d))) = w_H(bd)$,

If $b = d$, then $w_{G\times H}(((a, b),(c, d))) = w_G(ac)$.

In this section we compute the weighted Omega polynomial of Cartesian product of two weighted graphs.

Lemma 1. Let G and H be graphs. Then we have:

(a) $|V(G \times H)| = |V(G)|\,|V(H)|$,
$|E(G \times H)| = |E(G)|\,|V(H)| + |V(G)|\,|E(H)|$;
(b) $G \times H$ is connected if and only if G and H are connected;
(c) If (a, x) and (b, y) are vertices of G × H then

$$d_{G\times H}((a, x), (b, y)) = d_G(a, b) + d_H(x, y);$$

(d) the Cartesian product is associative.

We recall that for a graph G and $e \in E(G)$,

$$N(e) = |E| - (n_e u(e|G) + n_e v(e|G)).$$

The following result is direct consequence of Lemma 1.

Lemma 2. Suppose (a, x), (b, y) are adjacent vertices of $G \times H$, where G and H are co-graphs. Then

$$N_{G\times H}((a, x)(b, y)) = \begin{cases} |V(G)|\, N(f) & \text{for } a = b \text{ and } xy = f \in E(H) \\ |V(H)|\, N(g) & \text{for } x = y \text{ and } ab = g \in E(G) \end{cases},$$

$$w_{G\times H,e}(c) = \begin{cases} |V(G)|\, w_{H,e}(c) & \text{for } c = |V(G)|c_H \\ |V(H)|\, w_{G,e}(c) & \text{for } c = |V(H)|c_G \end{cases}.$$

Theorem 3. Let G and H be connected co-graphs. Then

Proof. By using Lemmas 1 and 2 and definition of Omega polynomial of a graph, we have:

$$\Omega_e(G\times H,x) = \sum_{c_1}\left[\frac{w_{G,e}(c_1)}{|c_1|}\right] m_1.x^{|V(H)|c_1} + \sum_{c_2}\left[\frac{w_{H,e}(c_2)}{|c_2|}\right] m_2.x^{|V(G)|c_2}$$

and

$$\begin{aligned}\Omega_e(G\times H,x) &= \sum_c m(G\times H,c).x^c \\ &= \sum_{c_1}\left[\frac{w_{G,e}(c_1)}{|c_1|}\right] m_1.x^{|V(H)|c_1} \\ &+ \sum_{c_2}\left[\frac{w_{H,e}(c_2)}{|c_2|}\right] m_2.x^{|V(G)|c_2}\end{aligned}$$

where, $m_1 = m(G,c_1)$, $m_2 = m(H,c_2)$ and this completes the proof.

Theorem 4. Let $G_1, G_2, \cdots, G_n$ be connected co-graphs. Then we have:

$$\Omega_e(G_1\times G_2\times\cdots\times G_n,x)=\sum_{i=1}^{n}\sum_{c_i}\left\lfloor\frac{w_{G_i,e}(c_i)}{|c_i|}\right\rfloor m(G_i,c_i).x^{\prod_{j=1,\,j\neq i}^{n}|V(G_j)|c_i}$$

Proof. We use induction on n. By Theorem 3, the result is valid for $n = 2$. Let $n \geq 3$ and assume the theorem holds for $n - 1$. Set $G = G_1\times\ldots\times G_{n-1}$. Then we have

$$\Omega_e(G\times G_n,x)=\sum_{c}\left\lfloor\frac{w_{G,e}(c)}{|c|}\right\rfloor m(G,c).x^{|V(G_n)|c}+\sum_{c_n}\left\lfloor\frac{w_{G_n,e}(c_n)}{|c_n|}\right\rfloor m(G_n,c_n).x^{|V(G)|c_n}$$

$$=\sum_{i=1}^{n-1}\sum_{c_i}\left\lfloor\frac{w_{G_i,e}(c_i)}{|c_i|}\right\rfloor m(G_i,c_i).x^{\prod_{j=1,\,j\neq i}^{n}|V(G_j)|c_i}+\sum_{c_n}\left\lfloor\frac{w_{G_n,e}(c_n)}{|c_n|}\right\rfloor m(G_n,c_n).x^{|V(G)|c_n}$$

$$=\sum_{i=1}^{n}\sum_{c_i}\left\lfloor\frac{w_{G_i,e}(c_i)}{|c_i|}\right\rfloor m(G_i,c_i).x^{\prod_{j=1,\,j\neq i}^{n}|V(G_j)|c_i}.$$

One can computes same results for the Sadhana and Theta polynomials as previously.

Examples

Example 1. Suppose Q_n denotes a hypercube of dimension n. Then by Theorem 2,

$$\Omega_e(Q_n,x)=\Omega_e(K_2^n,x)=n.\sum_{c}\left\lfloor\frac{w_{K_2,e}(c)}{|c|}\right\rfloor m(K_2,c).x^{|V(K_2)|^{n-1}c}.$$

$$=n.\lfloor w_e(K_2)\rfloor.x^{2^{n-1}}.$$

Example 2. Let P_n be a path of length n and C_n an n-cycle. Then

$$\Omega_e(C_n,x)=\begin{cases}\sum_{i=1}^{\frac{n}{2}}\left\lfloor\frac{w_{C_n,e}(c_i)}{2}\right\rfloor x^2 & 2|n\\ \sum_{i=1}^{n}\lfloor w_{C_n,e}(c_i)\rfloor x & 2\nmid n\end{cases}.$$

Also we have $\Omega_e(P_n,x)=\sum_{i=1}^{n-1}\left\lfloor w_{P_n,e}(c_i)\right\rfloor x$. So,

$$\Omega_e(P_n\times P_m,x)=\sum_{i=1}^{n-1}\left\lfloor w_{P_n,e}(c_i)\right\rfloor x^m+\sum_{j=1}^{m-1}\left\lfloor w_{P_n,e}(c_j)\right\rfloor x^n .$$

In the other words

$$\Omega_e(P_n\times C_m,x)=\begin{cases}\sum_{i=1}^{n-1}\left\lfloor w_{P_n,e}(c_i)\right\rfloor x^m+\sum_{j=1}^{\frac{m}{2}}\left\lfloor \frac{w_{C_m,e}(c_j)}{2}\right\rfloor x^{2n} & 2|m\\ \sum_{i=1}^{n-1}\left\lfloor w_{P_n,e}(c_i)\right\rfloor x^m+\sum_{j=1}^{m}\left\lfloor w_{C_m,e}(c_j)\right\rfloor x^{n} & 2\nmid m\end{cases},$$

$$\Omega_e(C_n\times C_m,x)=\begin{cases}\sum_{i=1}^{n}\left\lfloor w_{C_n,e}(c_i)\right\rfloor x^m+\sum_{j=1}^{m}\left\lfloor w_{C_m,e}(c_j)\right\rfloor x^{n} & 2\nmid m\ ,\ 2\nmid n\\ \sum_{i=1}^{n}\left\lfloor w_{C_n,e}(c_i)\right\rfloor x^m+\sum_{j=1}^{\frac{m}{2}}\left\lfloor \frac{w_{C_m,e}(c_j)}{2}\right\rfloor x^{2n} & 2|m\ ,\ 2\nmid n\\ \sum_{i=1}^{\frac{n}{2}}\left\lfloor \frac{w_{C_n,e}(c_i)}{2}\right\rfloor x^{2m}+\sum_{j=1}^{m}\left\lfloor w_{C_m,e}(c_j)\right\rfloor x^{n} & 2\nmid m\ ,\ 2|n\\ \sum_{i=1}^{\frac{n}{2}}\left\lfloor \frac{w_{C_n,e}(c_i)}{2}\right\rfloor x^{2m}+\sum_{j=1}^{\frac{m}{2}}\left\lfloor \frac{w_{C_m,e}(c_j)}{2}\right\rfloor x^{2n} & 2|m\ ,\ 2|n\end{cases}.$$

CONCLUSIONS

In this paper we defined three weighted versions of Omega, Theta and Sadhana polynomials and then we established some theoretical relations for them. We can apply the concept of weighted graph in molecular graph theory. The most important weight for edge/bond is the (covalent) bond length while for the vertex/atom, we can use the atomic radius, the partial charge in an optimized molecule by a quantum method, and so one. The topological indices derived from weighted polynomials, reflecting more properly the chemical characteristics of bonds/atoms, could be better used in QSAR/QSPR studies.

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