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OMEGA AND SADHANA POLYNOMIALS OF TWO CLASSES OF MOLECULAR GRAPHS

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ABSTRACT. The *Omega polynomial* of a connected graph *G*, denoted by $\Omega(G;x)$, is defined as $\Omega(G;x)=\sum_{c} m(G;c)x^{c}$ and the *Sadhana polynomial* of *G* is defined as $Sd(G;x)=\sum_{c} m(G;c)x^{|E(G)|-c}$, where *m(G; c)* is the number of strips of length *c* and *|E(G)|* is the number of edges in *G.* In this paper, we obtain explicit computing formulas for Omega and Sadhana polynomials of bridge graphs and chain graphs. As applications, Omega and Sadhana polynomials of some spiro-chains composed of four-member or six-member rings are deduced.

Keywords: *Quasi-ortogonal cut; Omega polynomial, Sadhana polynomial, bridge graph; chain graph*

INTRODUCTION

Let *G* denote a graph with vertex set *V(G)* and edge set *E(G)*. The distance between two vertices *x* and *y* in *V(G)*, denoted by *d(x,y)*, is equal to the length of the shortest path connecting *x* and *y*. Two edges *e=uv* and *f=xy* in *E(G)* are said to be *codistant*, denoted by *e co f*, if *d(x,u)= d(y,v)* and *d(x,v)= d(y,u)= d(x,u)+1= d(y,v)+1*. The relation"*co*" is reflexive, symmetric, but not necessarily transitive. Let $C(e)=\{f\in E(G): f$ *co e*}. If the relation „co" is transitive on *C(e)*, then *C(e) is* called an *orthogonal cut* „co" of the graph *G*.

Let *e=uv and f=xy* be two edges of a graph *G,* which are *opposite* or topological parallel, and this relation is denoted by *e op f*. A set of opposite edges, within the same face or ring, eventually forming a strip of adjacent

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faces/rings, is called an *opposite* edge *strip ops*, which is a quasi-ortogonal cut *qoc* (*i.e.*, the transitivity relation is not necessarily obeyed). Note that the „*co”* relation is defined in the whole graph while the relation „*op”* is defined only in a face/ring. We will always assume that the length of *ops* is maximal irrespective of the starting edge.

Let *m(G; c)* be the number of *ops* strips of length *c*. The Omega polynomial of a connected graph *G*, denoted by $\Omega(G;x)$, is then defined as [1, 2]: $\Omega(G;x)=\sum_c m(G;c)x^c$ and the Sadhana polynomial of *G* is defined as [3]: $Sd(G;x)=\sum_c m(G;c)x^{|E(G)|-c}$, where *|E(G)|* is the number of edges in *G*. For recent results concerning the above two computing polynomials, the reader is referred to [4-11] and the references cited therein.

In this paper, we obtain Omega and Sadhana polynomials for the bridge graphs and chain graphs. As applications, Omega and Sadhana polynomials of some spiro-chains composed of four-member or six-member rings are obtained.

RESULTS AND DISCUSSION

In this section, we shall compute the Omega and Sadhana polynomials for the bridge graphs and chain graphs ([see, 12,13]). Let G_1, G_2,…, G_d be a set of finite pairwise disjoint graphs with $v_i \in V(G_i)$. The *bridge graph* $G = B(G_1, G_2,...G_d; v_1, v_2,...v_d)$ is obtained by connecting the vertices v_i and v_{i+1} by an edge for each *i=1, 2,..,d-1*, see Figure. 1.

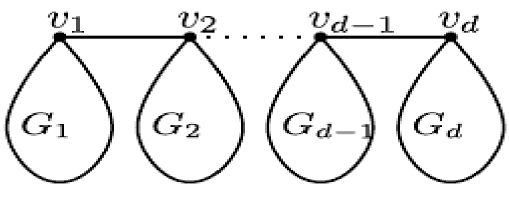

Figure1. The bridge graph $G = B(G_1, G_2,...G_d; v_1, v_2,...v_d)$.

The following theorem give the formulas for Omega and Sadhana polynomials of the bridge graphs.

Theorem 1. *Let* $G = B(G_1, G_2, ...G_d; v_1, v_2, ...v_d)$ *be the bridge graph with m edges, as shown in Figure1. Suppose that each* G_i has m_i edges. *Then*

$$\begin{aligned}\Omega(G;x) &= \sum_c m(G;c)x^c \\ &= \Omega(G_1;x) + \ldots + \Omega(G_d;x) + (d-1)x\end{aligned}$$

and

$$\begin{aligned}Sd(G;x) &= \sum_c m(G;c)x^{|E(G)|-c} \\ &= x^{m-m_1}Sd(G_1;x) + x^{m-m_2}Sd(G_2;x) + \ldots + \\ &\quad x^{m-m_d}Sd(G_d;x) + (d-1)x^{m-1}.\end{aligned}$$

Proof. Suppose that S_c is a strip of length *c* in G. If $c \geq 2$, then S_c lies entirely within some $G_i (1 \leq i \leq d)$. Suppose to the contrary that there are two edges *e* and *f* in S_c satisfying that *e* belongs to some given G_i, but *f* does not belong to G_i. But then two edges *e* and *f* can not be topological parallel to each other, a contradiction. That is, S_c lies entirely within some $G_i (1 \leq i \leq d)$. By the same reasoning, we know that there exists no other edges can be added into this strip such that we can get a new strip of length greater than c. By these arguments, we claim that the number of strips in G of length $c \geq 2$ does not change. So we have

$$\begin{aligned}\Omega(G;x) &= \sum_c m(G;c)x^c \\ &= \Omega(G_1;x) + \ldots + \Omega(G_d;x) + (d-1)x.\end{aligned}$$

Note that for each strip S_c of length c in some G_i, we have $m(G;c) = m(G_i;c)$ (not including the case of $c = 1$) and $x^{|E(G)|-c} = x^{m-m_i} x^{m_i - c}$. Thus,

$$\begin{aligned}Sd(G;x) &= \sum_c m(G;c)x^{|E(G)|-c} \\ &= x^{m-m_1}Sd(G_1;x) + x^{m-m_2}Sd(G_2;x) + \ldots + \\ &\quad x^{m-m_d}Sd(G_d;x) + (d-1)x^{m-1}.\end{aligned}$$

This completes the proof.

If we let $G_i = H$ and $v_i = v$ for each *i=1,2,…d* in above theorem, we immediately have the following result. In this case, for each *i=1,2,…d,* $m_i = \frac{m-d+1}{d}$.

Corollary 1. *Let* $G = B(H, H, ...H; v, v, ...v)$ *(d times) be the bridge graph with m edges, as shown in Figure 1. Then*

$$\begin{aligned}\Omega(G;x) &= \sum_c m(G;c)x^c \\ &= d\Omega(H;x) + (d-1)x\end{aligned}$$

and

$$\begin{aligned}Sd(G;x) &= \sum_c m(G;c)x^{|E(G)|-c} \\ &= x^{m-\frac{m-d+1}{d}}[d \cdot Sd(H;x)] + (d-1)x^{m-1} \\ &= d \cdot x^{\frac{(m+1)(d-1)}{d}} Sd(H;x) + (d-1)x^{m-1}.\end{aligned}$$

Now, we consider some examples of bridge graphs.

Figure 2. The graph $B_{d,3}$.

Example 1. Consider the bridge graph $B_{d,3} = (P_3, P_3, ...P_3; v, v, ...v)$ (*d* times), where P_3 is the 3-vertex path with the middle vertex being *v,* see Figure 2. Note that $\Omega(P_3; x) = 2x$ and $Sd(P_3; x) = 2x$. Then by Corollary 1, we obtain $\Omega(B_{d,3};x) = d \cdot (2x) + (d-1)x = (3d-1)x$ and

$$Sd(B_{d,3}; x) = x^{3(d-1)} \cdot d \cdot (2x) + (d-1)x^{3d-2} = (3d-1)x^{3d-2}.$$

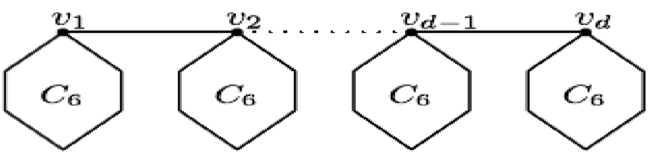

Figure 3. The bridge graph of the hexagon C_6.

Example 2. Consider the bridge graph $G = B(C_6, C_6, ...C_6)$ (*d* times), see Figure 3. Note that $\Omega(C_6; x) = 3x^2$ and $Sd(C_6; x) = 3x^4$. Then by Corollary 1, we obtain $\Omega(B(C_6, C_6, ..C_6; v_1, v_2, .., v_d); x) = 3dx^2 + (d-1)x$ and $Sd(B(C_6, C_6, ..C_6; v_1, v_2, .., v_d); x) = x^{7(d-1)} \cdot 3dx^4 + (d-1)x^{7d-2} = 3dx^{7d-3} + (d-1)x^{7d-2}$.

Let G_1, G_2,..., G_d be a set of finite pairwise disjoint graphs with $v_i, w_i \in V(G_i)$. The *chain graph* $C(G_1, G_2, ...G_d; v_1, w_1, v_2, w_2, ..., v_d, w_d)$ is obtained by identifying the vertex w_i and the vertex v_{i+1} for each *i=1, 2,..,d-1*, see Figure 4.

Figure 4. The chain graph $C(G_1, G_2, ...G_d; v_1, w_1, v_2, w_2, ..., v_d, w_d)$.

Theorem 2. *Let* $G = C(G_1, G_2, ...G_d; v_1, w_1, v_2, w_2, ..., v_d, w_d)$ *be the chain graph with m edges, as shown in Figure 2. Suppose that each* G_i has m_i edges. *Then*

$$\Omega(G; x) = \sum_c m(G; c)x^c = \Omega(G_1; x) + \ldots + \Omega(G_d; x)$$

and

$$Sd(G; x) = \sum_c m(G; c)x^{|E(G)|-c} = x^{m-m_1} Sd(G_1; x) + x^{m-m_2} Sd(G_2; x) + \ldots + x^{m-m_d} Sd(G_d; x).$$

Proof. Suppose that S_c is a strip of length *c* in G. If $c \geq 2$, then S_c lies entirely within some $G_i (1 \leq i \leq d)$. Also, there is no other edges can be added into this strip such that we can get a new strip of length greater than c. By these arguments, we thus have

$$\begin{aligned}\Omega(G;x) &= \sum_c m(G;c)x^c \\ &= \Omega(G_1;x)+\ldots+\Omega(G_d;x)\end{aligned}$$

and

$$\begin{aligned}Sd(G;x) &= \sum_c m(G;c)x^{|E(G)|-c} \\ &= x^{m-m_1}Sd(G_1;x)+x^{m-m_2}Sd(G_2;x)+\ldots+ \\ &\quad x^{m-m_d}Sd(G_d;x).\end{aligned}$$

This completes the proof.

If we set $G_i = H$ and $v_i = v$ for each *i=1,2,…d* in Theorem 2, we immediately have the following result.

Corollary 2. *Let* $G = C(H, H, \ldots H; v, v, \ldots v)$ *(d times) be the chain graph. Then*

$$\begin{aligned}\Omega(G;x) &= \sum_c m(G;c)x^c \\ &= d\Omega(H;x)\end{aligned}$$

and

$$\begin{aligned}Sd(G;x) &= \sum_c m(G;c)x^{|E(G)|-c} \\ &= dx^{m-\frac{m}{d}}Sd(H;x) \\ &= dx^{\frac{(d-1)m}{d}}Sd(H;x).\end{aligned}$$

Now, we consider some examples of chain graphs as shown in Figures 5-7.

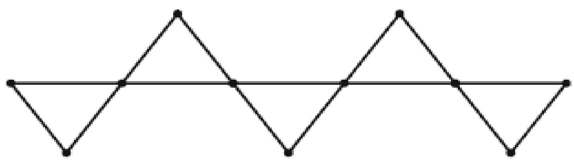

Figure 5. The spiro-chain graph of C_3 with d=5.

Figure 6. The spiro-chain graph $C_4(1,3)$.

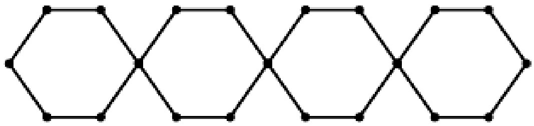

Figure 7. The spiro-chain graph $C_6(1,4)$ with d=4.

Example 3. Consider the spiro-chain graph as shown in Figure 5. Note that $\Omega(C_3;x)=3x$ and $Sd(C_3;x)=3x^2$. Then by Corollary 2, we obtain $\Omega(G;x)=15x$ and $Sd(B(C_6,C_6,...C_6);x)=15x^{14}$.

Example 4. Consider the spiro-chain graph as shown in Figure 6. Note that $\Omega(C_4;x)=2x^2$ and $Sd(C_4;x)=2x^2$. Then by Corollary 2, we obtain $\Omega(G;x)=2dx^2$ and $Sd(G;x)=2dx^{4d-2}$.

Example 5. Consider the spiro-chain graph as shown in Figure 7. Note that $\Omega(C_6;x)=3x^2$ and $Sd(C_3;x)=3x^4$. Then by Corollary 2, we obtain $\Omega(G;x)=12x^2$ and. $Sd(G;x)=12dx^{22}$.

CONCLUSIONS

In this paper, we obtained explicit computing formulas for Omega and Sadhana polynomials of bridge graphs and chain graphs. As applications, Omega and Sadhana polynomials of some spiro-chains composed of four-member or six-member rings are deduced. It may be interesting to investigate Omega and Sadhana polynomials for other molecular graphs and nanostrutures.

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