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Omega and Related Counting Polynomials

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Abstract. Counting polynomials are those polynomials having at exponent the extent of a property partition and coefficients the multiplicity/occurrence of the corresponding partition. In the present paper three related counting polynomials are discussed: Omega Ω, Equidistance Θ and Non-Equidistance Π polynomials, and their mutual inter-relations in some particular graphs and lattices, as well. Analytical close formulas for some cubic lattices and their corresponding cages are derived.

1. Counting Polynomials

A graph can be described by a connection table, a sequence of numbers, a matrix, a polynomial or a derived unique number (often called a topological index). In Quantum Chemistry, the early Hückel theory calculates the levels of π-electron energy of the molecular orbitals, in conjugated hydrocarbons, as roots of the *characteristic polynomial*:[1-4]

$$P(G,x) = \det[x\mathrm{I} - \mathrm{A}(G)] \tag{1}$$

In the above, I is the unit matrix of a pertinent order and A the adjacency matrix of the graph *G*. The characteristic polynomial is involved in the evaluation of topological resonance energy TRE, the topological effect on molecular orbitals TEMO, the aromatic sextet theory, the Kekulé structure count, etc.[4-8]

The coefficients $m(G,k)$ in the polynomial expression:

$$P(G,x)=\sum_k m(G,k)\cdot x^k \qquad (2)$$

are calculable from the graph *G* by a method making use of the *Sachs graphs*, which are subgraphs of *G*. Relation (2) was found independently by Sachs, Harary, Milić, Spialter, Hosoya, *etc*.[1] The above method is useful in small graphs but, in larger ones, the numeric methods of linear algebra, such as the recursive algorithms of Le Verier, Frame, or Fadeev, are more efficient.[9,10]

An extension of relation (1) was made by Hosoya[11] and others[12-15] by changing the adjacency matrix with the distance matrix and next by any square topological matrix.

Relation (2) is a general expression of a counting polynomial, written as a sequence of numbers, with the exponents showing the extent of partitions $p(G)$, $\cup\, p(G)=P(G)$ of a graph property $P(G)$ while the coefficients $m(G,k)$ are related to the occurrence/multiplicity of partitions of extent *k*.

Counting polynomials are related, in the Mathematical Chemistry literature, to the name of Hosoya:[16,17] independent edge sets are counted by $Z(G,x)$ and distances counted by $H(G,x)$ (initially called Wiener and later Hosoya)[18,19] polynomials. Their roots and coefficients are used for the characterization of topological nature of hydrocarbons. Hosoya also proposed the sextet polynomial[20-23] for counting the resonant rings in a benzenoid molecule. The sextet polynomial is important in connection with the Clar aromatic sextets,[24,25] expected to stabilize the aromatic molecules.

The independence polynomial[26-28] counts selections of *k*-independent vertices of *G*. Other related graph polynomials are the *king*, *color*, *star* or *clique polynomials*.[29-33] More about polynomials the reader can find in ref 1.

Some distance-related properties can be expressed in polynomial form, with coefficients calculable from the layer and shell matrices.[34-38] These matrices are built up according to the vertex distance partitions of a graph, as provided by the TOPOCLUJ software package.[39] The most important, in this respect, is the evaluation of the coefficients of Hosoya $H(G,x)$ polynomial from the layer of counting LC matrix.[36,37]

The aim of this paper is to clarify the relation of Omega with other two counting polynomials and to present new close formulas for calculating Omega polynomial in some 3D infinite networks.

2. Definitions

Let *G*(*V*,*E*) be a connected bipartite graph, with the vertex set *V*(*G*) and edge set *E*(*G*). Two edges *e* = (*u*,*v*) and *f* = (*x*,*y*) of *G* are called *codistant* (briefly: *e co f*) if

$$d(v,x) = d(v,y)+1 = d(u,x)+1 = d(u,y) \qquad (3)$$

For some edges of a connected graph *G* there are the following relations satisfied:[40,41]

$$e\ co\ e \qquad (4)$$

$$e\ co\ f \Leftrightarrow f\ co\ e \qquad (5)$$

$$e\ co\ f\ \&\ f\ co\ h \Rightarrow e\ co\ h \qquad (6)$$

though the relation (6) is not always valid (Figure 1 and Table 1).

Let $C(e) := \{f \in E(G);\ f\ co\ e\}$ denote the set of edges in *G*, codistant to the edge $e \in E(G)$. If relation *co* is an equivalence relation (*i.e.*, all the elements of *C*(*e*) satisfy the relations (4) to (6), then *G* is called a *co-graph* . Consequently, *C*(*e*) is called an *orthogonal cut oc* of *G* and *E*(*G*) is the union of disjoint orthogonal cuts: $C_1 \cup C_2 \cup ... \cup C_k$ and $Ci \cap Cj = \emptyset$ for $i \neq j,\ i, j = 1,2,..,k$.

Observe *co* is a θ relation, (Djoković-Winkler relation) and θ *is a co-graph if and only if G is a partial cube,* as Klavžar[42] correctly stated in a recent paper, dedicated to our *CI* index (see below). In this respect, recall some basic definitions (Ovchinikov[43]).

A subgraph $H \subseteq G$ is called *isometric*, if $d_H(u,v) = d_G(u,v)$, for any $(u,v) \in H$; it is *convex* if any shortest path in *G* between vertices of *H* belongs to *H*. A *partial cube* is a graph that can be isometrically embedded into a *hypercube* $\mathcal{H}(X)$, which vertices are finite subsets $P_f(X)$ of *X*. A pair of such subsets (*A*,*B*) is an edge of $\mathcal{H}(X)$ if the symmetric difference $A\Delta B$ is a singleton. The graph $\mathcal{H}(X)$ is called the hypercube on *X*. The dimension of $\mathcal{H}(X)$ is the cardinality of the set *X*. The shortest path *d*(*A*,*B*) on $\mathcal{H}(X)$ is the Hamming distances between subsets *A* and *B*: $d(A,B) = |A\Delta B|$. The set $P_f(X)$ is a metric space with the metric *d*.

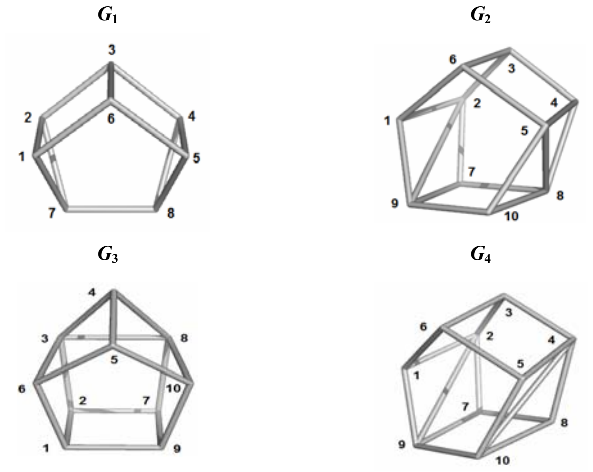


Figure 1. Cuneane $\boldsymbol{G_1}$ and its derived graphs $\boldsymbol{G_2}$ to $\boldsymbol{G_4}$.

$\boldsymbol{G_1}$: the equidistant (see below) edges 3-6 and 7-8 do not belong to the same face/ring, so they do not belong to a strip in $\Omega(G,x)$, the last one being counted by the term of exponent unity (together with 1-7, 2-7, 4-8 and 5-8). $\boldsymbol{G_2}$ and $\boldsymbol{G_4}$ show the same strips in $\Omega(G,x)$ and correspondingly degenerate polynomial, while different $\Theta(G,x)$ and $\Pi(G,x)$. All the graphs show distinct $\Theta(G,x)$ and $\Pi(G,x)$ polynomials.

Let $G(V,E)$ be a connected graph and d be its distance function. For any two adjacent vertices $(a,b) \in E(G)$, let denote by W_{ab}, the set of vertices lying closer to a than to b: $W_{ab} = \{w \in V \mid d(w,a) < d(w,b)\}$. The set W_{ab} and its induced subgraphs $\langle W_{ab} \rangle$ are called *semicubes* of G. The semicubes W_{ab} and W_{ba} are called opposite semicubes. Two opposite semicubes are disjoint. A graph G is bipartite if and only if its semicubes W_{ab} and W_{ba} form a partition of V for any $(a,b) \in E(G)$. Let $w \in W_{ab}$ for some edge $(a,b) \in E(G)$. Then $d(w,b) = d(w,a) + 1$ and consequently $W_{ab} = \{w \in V \mid d(w,b) = d(w,a) + 1\}$.

If $G(V,E)$ is a connected graph and $e = (u,v)$ and $f = (x,y)$ are two edges of G, a relation θ on $E(G)$ can be defined (Djoković[44]) as:

$$e\,\theta\,f \Leftrightarrow f \textit{ joins a vertex in } W_{xy} \textit{ with a vertex in } W_{yx} \tag{7}$$

We can change the notation such that $u \in W_{xy}$ and $v \in W_{yx}$.

Winkler[45] has defined a different relation Θ on $E(G)$ as:

$$e\,\Theta f \Leftrightarrow d(u,x) + d(v,y) \neq d(u,y) + d(v,x) \tag{8}$$

In general, $\theta \subseteq \Theta$ while a graph *G* is bipartite if and only if $\theta = \Theta$. In a bipartite graph, all semicubes are convex and the relation θ is an equivalence relation on *E*. A partial cube is just a bipartite graph, having all of its semicubes convex subsets of *V*, each pair of opposite semicubes forming a partition of *V* and θ is an equivalence relation on *E*. In a partial cube, for any pair of adjacent vertices of G, there is a unique pair of opposite semicubes separating the two vertices. From the above statements, we also can write: $d(v,x) = d(v,y) + 1 = d(u,y)$.

The isometric dimension $dim_I(G)$ of a partial cube *G* is the smallest dimension of a hypercube H(*X*) in which G is isometrically embeddable. It can be evaluated as:

$$\dim_I(G) = |E/\theta| \qquad (9)$$

where E/θ is the set of its equivalence classes, also called the *Θ-classes* of *G*. The edges in each class are parallel to each other.

It is now clear that the relation *co* is a relation *Θ*. In a plane bipartite graph, an edge *f* is in relation *Θ* with any opposite edge *e* if the faces of the plane graph are isometric (which is the case of the most chemical graphs). Then an orthogonal cut *oc* with respect to a given edge is the smallest subset of edges closed under this operation and *C*(e) is precisely a *Θ*-class of *G*. Concluding, a *graph G is a co-graph if and only if it is a partial cube.* Note that Cluj polynomial[46] is based on calculation of opposite semicubes (non-equidistant vertices).

Table 1. Counting polynomials of Cuneane and its derived graphs in Figure 1.

	Omega	Theta	PI
G_1	$5x + 2x^2 + x^3$	$4x + 5x^2 + 2x^3 + x^4$	$x^8 + 2x^9 + 5x^{10} + 4x^{11}$
e=12	CI=122	Θ'=24	PI=120
G_2	$6x + 4x^2 + x^3$	$2x + 6x^2 + 7x^3 + 2x^4 / wct$	$2x^{13} + 7x^{14} + 6x^{15} + 2x^{16} / wct$
e=17	CI=258	Θ'=43	PI=246
		$2x + 12x^2 + x^3 + 2x^4 / cut$	$2x^{13} + x^{14} + 12x^{15} + 2x^{16} / cut$
		Θ'=37	PI=252
G_3	$2x^2 + x^3 + x^4 + x^5$	$4x^2 + 5x^3 + 4x^4 + 3x^5 / wct$	$3x^{11} + 4x^{12} + 5x^{13} + 4x^{14} / wct$
e=16	CI=198	Θ'=54	PI=202
		$4x^2 + 8x^3 + 2x^4 + 2x^5 / cut$	$2x^{11} + 2x^{12} + 8x^{13} + 4x^{14} / cut$
		Θ'=50	PI=206
G_4	$6x + 4x^2 + x^3$	$2x + 7x^2 + 7x^3 + x^4$	$x^{13} + 7x^{14} + 7x^{15} + 2x^{16}$
e=17	CI=258	Θ'=41	PI=248

If any two consecutive edges of an edge-cut sequence are *opposite*, or *topologically parallel* within the same face/ring of the covering/tiling, such a sequence is called a *quasi-orthogonal cut qoc* strip. This means the transitivity relation (6) of the *co* relation is not necessarily obeyed. Any *oc* strip is a *qoc* strip but the reverse is not always true.[47,48]

3. Omega-type Polynomials

Let $m(G,c)$ be the number of *qoc* strips of length c (*i.e.*, the number of cut-off edges); for the sake of simplicity, $m(G,c)$ will hereafter be written as m. Three counting polynomials can be defined,[49] in simple bipartite planar graphs (e.g., acenes, fenacenes), on the ground of *qoc* strips:

$$\Omega(G,x) = \sum_c m \cdot x^c \tag{10}$$

$$\Theta(G,x) = \sum_c m \cdot c \cdot x^c \tag{11}$$

$$\Pi(G,x) = \sum_c m \cdot c \cdot x^{e-c} \tag{12}$$

Omega and Theta polynomials count *equidistant edges* in G while *PI* polynomial, non-equidistant ones. Note that Ashrafi *et al.*[50] have firstly proposed $\Pi(G,x)$, (written as PI(G,x)), to account for the Khadikar's $PI=PI(G)$ topological index[51] (see below). Theta polynomial is presented here for the first time.

Note that *edge equidistance* relation includes *co* relation; to check the equidistant edges, the following relation, true in case of non-opposite edges, is added to (3):

$$d(u,x) = d(u,y) = d(v,x) = d(v,y) \tag{13}$$

In this respect, edges 3-6 and 7-8 of $\boldsymbol{G_1}$ (Figure 1) are equidistant.

In a counting polynomial, the *first derivative* (in x=1) $\mathrm{D1}|_{x=1}$, defines the type of property which is counted; for the three polynomials they are:

$$\Omega'(G,x)_{|x=1} = \sum_c m \cdot c = e = |E(G)| \tag{14}$$

$$\Theta'(G,x)_{|x=1} = \sum_c m \cdot c^2 = \theta(G) \tag{15}$$

$$\Pi'(G,x)_{|x=1} = \sum_c m \cdot c \cdot (e-c) = PI(G) \tag{16}$$

Reformulating (16) function of (10) and (11) we can write:

$$PI(G) = e^2 - \sum_c m \cdot c^2 = \{[\Omega'(G,x)]^2 - \Theta'(G,x)\}_{|x=1} \tag{17}$$

The first part of relation (17) is just the formula proposed by John *et al.*[40] to calculate the *PI* index (see also ref. 52).

On the other hand, the Cluj-Ilmenau[41] index, $CI = CI(G)$, is calculable from Omega[49] polynomial as:

$$CI(G) = \left\{[\Omega'(G,x)]^2 - [\Omega'(G,x) + \Omega''(G,x)]\right\}_{|x=1} \tag{18}$$

It is easily seen that, for a single *qoc*, one calculates the polynomial: $\Omega(G,x) = 1 \times x^c$ and $CI(G) = c^2 - (c + c(c-1)) = c^2 - c^2 = 0$.

Proposition. *There exist bipartite planar graphs for which CI=PI.*

Applying definition (18), *CI* is calculated as:

$$CI(G) = \left(\sum_c m\cdot c\right)^2 - \left[\sum_c m\cdot c + \sum_c m\cdot c\cdot(c-1)\right] = e^2 - \sum_c m\cdot c^2 = PI(G) \tag{19}$$

There are graphs (bipartite, like C_{cage}, Figure 2a, or non-bipartite, like those in Figure 1 and Table 1) where $\Theta(G,x)$ and $\Pi(G,x)$, respectively, show different expressions, function of the manner of distance counting: (i) within the subgraph G_{cut} obtained by cutting-off the two edges searched for equidistance (denoted *cut*) or (ii) within *G* (denoted *no cut*).

The two indices *CI* and *PI* show identical values if the subgraphs G_{cut} corresponding to all pair edges in *G*, are isometric to *G*. In such cases, the two distance counting methods give one and the same result.

As clear examples, the bipartite planar graphs of acenes and phenacenes are given in Table 2. Analytical formulas[53] for the Omega and related polynomials, in these two classes of polyhex molecular graphs are given in Tables 3 and 4.

Table 2. Counting polynomials in acenes A_n, and phenacenes Ph_n

	Omega	CI	$\Theta(G,x)$	θ	$\Pi(G,x)$	PI
A3	$6x^2+x^4$	216	$12x^2+4x^4$	40	$4x^{12}+12x^{14}$	216
A4	$8x^2+x^5$	384	$16x^2+5x^5$	57	$5x^{16}+16x^{19}$	384
Ph3	$5x^2+2x^3$	218	$10x^2+6x^3$	38	$6x^{13}+10x^{14}$	218
Ph4	$6x^2+3x^3$	390	$12x^2+9x^3$	51	$9x^{18}+12x^{19}$	390

Table 3. Formulas for Omega-type polynomials in acenes A_h; h = no. hexagons in *G*.

$\Omega(A_h,x) = 2h\cdot x^2 + x^{(h+1)}$; $|D1|_{x=1} = e = 5h+1$; $D2|_{x=1} = h(h+5)$

$CI(A_h) = (\Omega'(A_h))^2 - (\Omega'(A_h) + \Omega''(A_h)) = (5h+1)^2 - (5h+1+h(h+5)) = 24h^2$

$\Omega(A_h,x)|_{x=1} = v/2 = 2h+1$

$\Pi(A_h,x) = 4h\cdot x^{5h-1} + (h+1)\cdot x^{4h}$; $D1|_{x=1} = 24h^2$

$\Theta(A_h,x) = 4h\times x^2 + (h+1)\times x^{h+1}$; $D1|_{x=1} = h^2+10h+1$

Table 4. Formulas for Omega-type polynomials in phenacenes Ph_h ; h = no. hexagons in G

$\Omega(Ph_h, x) = (h+2)\cdot x^2 + (h-1)\cdot x^3;\ D1\|_{x=1} = e = 5h+1;\ D2\|_{x=1} = 8h-2$
$CI(Ph_h) = (5h+1)^2 - (5h+1+8h-2) = 25h^2 - 3h + 2$
$\Omega(Ph_h, x)\|_{x=1} = v/2 = 2h+1$
$\Pi(Ph_h, x) = 2(h+2)\cdot x^{5h-1} + 3(h-1)\cdot x^{5h-2};\ D1\|_{x=1} = 25h^2 - 3h + 2$
$\Theta(Ph_h, x) = 2(h+2)\cdot x^2 + 3(h-1)\cdot x^3;\ D1\|_{x=1} = 13h - 1$

Other example is the *pcu* cubic lattice C_{net} (Figure 2b), which is precisely a partial cube (in our terms, *a co-graph*) and the strips represent orthogonal cuts *oc*; it means that all the three relations (10) to (12) are valid, and G_{cut}`s are isometric to G, such that *CI=PI.* At this stage, we cannot, however, give a general rule for the isometricity. Note that, in Ref. 53, $\Pi(G,x)$ was denoted by $N\Omega(G,x)$.

(a) $C(2,2,2)_{cage}$: $v = 26$; $e = 48$; f_4=24

$\Omega(G,x) = 6x^8$; CI=1920

$\Theta(G,x) = 24x^8 + 24x^{10}$; Θ' =432; no cut

$\Theta(G,x) = 24x^8 + 24x^9$; Θ' =408; cut

$\Pi(G,x) = 24x^{38} + 24x^{40}$; PI=1872; no cut

$\Pi(G,x) = 24x^{39} + 24x^{40}$; PI=1896; cut

(b) $C(2,2,2)_{net}$; $v = 27$; $e = 54$; r_4=36

$\Omega(G,x) = 6x^9$; ***CI* =2430**

$\Theta(G,x) = 54x^9$; Θ' =486

$\Pi(G,x) = 54x^{45}$; ***PI* =2430**

Figure 2. A planar bipartite cage and its corresponding bipartite net

Comparing (17) and (18) it is evident that:

$$\Theta'(G) = [\Omega'(G,x) + \Omega''(G,x)]_{|x=1} \tag{20}$$

In the above, the following relations hold:

$$e(G) = \sum_c m\cdot c = \Omega'(G,x)_{|x=1} = \Theta(G,x)_{|x=1} \tag{21}$$

From relations (17) and (21), $PI(G)$ can be calculated function of the only Theta polynomial:

$$PI(G) = \left\{[\Theta(G,x)]^2 - \Theta'(G,x)\right\}_{|x=1} \qquad (22)$$

There exist bipartite non-planar graphs (of genus *g*>0, e.g., square tiled torus TW0D[6,10]; Table 5: row 1) for which $CI \neq PI$. Conversely, there exist non-bipartite non-planar graphs with *CI=PI* (TWV3D[6,10]; Table 5, row 7), in this last case $c = c_\Theta$ (see below). There exist graphs for which the discussed indices show degenerate values: for *CI* see Table 1, G_2 and G_4 and Table 5 (rows 2 and 4, with degenerate both polynomial and single number index). In case of *PI* index, Table 5 (rows 2 and 6) shows degenerate index values (in italics) but distinct polynomials.

Table 5. Polynomials in square tiled (4,4) tori: a bipartite graph for which $CI \neq PI$ (row 1) and a non-bipartite graph showing *CI=PI* (row 7).

	Torus	Omega		Theta		PI
	(4,4)		CI		PI	
1	TW0D[6,10]	$10x^6+6x^{10}$	13440	$60x^{12}+60x^{20}$	12480	$60x^{100}+60x^{108}$
2	**TWH2D[6,10]**	***$6x^{10}+2x^{30}$***	***12000***	$60x^{18}+60x^{24}$	***11880***	$60x^{96}+60x^{102}$
3	TWH3D[6,10]	$6x^{10}+x^{60}$	10200	$120x^{10}$	13200	$120x^{110}$
4	**TWH6D[6,10]**	***$6x^{10}+2x^{30}$***	***12000***	$60x^{26}+60x^{28}$	11160	$60x^{92}+60x^{94}$
5	TWV1D[6,10]	$10x^6+x^{60}$	10440	$60x^6+60x^{18}$	12960	$60x^{102}+60x^{114}$
6	TWV2D[6,10]	$10x^6+2x^{30}$	12240	$60x^{16}+60x^{26}$	***11880***	$60x^{94}+60x^{104}$
7	**TWV3D[6,10]**	**$10x^6+3x^{20}$**	**12840**	**$60x^6+60x^{20}$**	**12840**	**$60x^{100}+60x^{114}$**

Despite relations (11) and (12) are not valid in general, relation (22) is still true. The two polynomials can be re-written as:

$$\Theta(G,x) = \sum\nolimits_c m_\Theta(G,c_\Theta) \cdot x^{c_\Theta} \qquad (11`)$$

$$\Pi(G,x) = \sum\nolimits_c m_\Theta(G,c_\Theta) \cdot x^{e-c_\Theta} \qquad (12`)$$

where c_Θ has now the meaning of cardinality of sets of equidistant edges. From the complementariness of equidistant/non-equidistant edges in *G*, it follows that the two polynomials have the same coefficients but complementary (to *e*) exponents. The Khadikar's index *PI* can thus be calculated from either of the two polynomials (relations (17) and (22)), for any graph.

The major difference between Omega and Theta polynomials is the first one excludes the already cut edge to the further cuttings. This is not the case for the Theta polynomial, but in planar bipartite graphs its coefficients can be calculated from the coefficients of $\Omega(G,x)$ by simply multiplying by *c*.

In tree graphs, the Omega polynomial is either not defined or it simply counts the non-equidistant edges as self-equidistant ones, being included in the term of exponent c=1. In such graphs, CI=PI =(v-1)(v-2) (a result known from Khadikar[54]) and the Omega and Theta polynomials show the same expression (compare (10) and (11`).

The coefficient of the term of exponent c=1 has found utility as a topological index, called n_p, the number of *pentagon fusions*, appearing in small fullerenes as a destabilizing factor. This index accounts for more than 90 % of the variance in heat of formation HF of fullerenes C_{40} and C_{50}.[55]

The following tables give examples for the three polynomials and derived numbers and formulas for counting their expressions: Tables 6 and 7 list data for the cubic cage C_{cage} (Figure 2a) and its medial transform. Tables 8 and 9 include data for the cubic net C_{net} (Figure 2b) and its medial *Med*(C_{net}) (Figure 3a). Note that the bipartite net C_{net} can be represented as the Cartesian product of three copies of the path on three vertices. Formula for the PI index of such a net is also given in ref. 52. Table 9 also gives formula for counting Omega polynomial in *Med*(*Med*(OP))$CO_{60,net}$ (Figure 3b), which is a unit of an infinite spongy network.

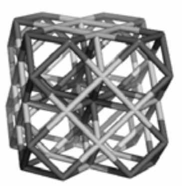
Table 6. Counting polynomials in $C(a,a,a)_{cage}$

	Omega	Theta	PI
a=1 v=8 e=12	$3x^4$ CI=96	$12x^4$ Θ'=48	$12x^8$ PI=96
a=2 v=26 e=48	$6x^8$ CI=1920	$24x^8+24x^9$ cut $24x^8+24x^{10}$ nocut Θ'=408cut/432 no cut	$24x^{40}+24x^{39}$ cut $24x^{40}+24x^{38}$ no cut PI=1896cut/1872 no cut
a=3 v=64 e=108	$9x^{12}$ CI=10368	$60x^{12}+48x^{14}$ cut $60x^{12}+48x^{16}$ no cut Θ'=1392/1488	$60x^{96}+48x^{94}$ cut $60x^{96}+48x^{92}$ no cut PI=10272cut/10176 no cut
a=4 v=98 e=192	$12x^{16}$ CI=33792	$96x^{16}+24x^{17}+48x^{20}+24x^{22}$ cut $96x^{16}+24x^{18}+72x^{22}$ no cut Θ'=3432/3552	$96x^{176}+24x^{175}+48x^{172}+72x^{170}$ cut $96x^{176}+24x^{174}+72x^{170}$ no cut PI=33432cut/33312 no cut

Table 7. Formulas for Omega polynomial in $C(a,a,a)_{cage}$ and its medial.

$C(a,a,a)_{cage}$
$v(C(a,a,a)_{cage})=(a+1)^3-(a-1)^3$; $c=4a$; $m=3a$; a – no. of squares in a $C(a,a,a)_{cage}$
$\Omega(C(a,a,a)_{cage},x)=3a\cdot x^{4a}$
***Med*(C(*a*,*a*,*a*)$_{cage}$)**
$\Omega(Med(C(a,a,a)_{cage}),x)=12x^{2a}+4x^{6a}$

(a) $Med(C(a,a,a)_{net})$; $a=2$; $v=54$
$\Omega(G,x)=36x^2+18x^4$
$CI=20304$; $PI=17712$



(b) $Med(Med(OP))CO_{60}(a,a,a)$; $a=1$; $v=60$
$\Omega(G,x)=24x^2+12x^3+18x^4$
$CI=23844$; $PI=21384$

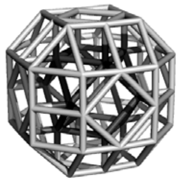


Figure 3. Graphs showing $CI \neq PI$

Table 8. Data for the three polynomials in the cubic *pcu* net $C(a,a,a)_{net}$

Cubic Net	Omega	Theta	PI	D1 Ratios
a=1 v=8 e=12	$3x^4$ CI=96	$12x^4$ Θ'=48	$12x^8$ Π'=96	Π'/Θ'=2 Π'/Ω'=8 Θ'/Ω'=4
a=2 v=27 e=54	$6x^9$ CI=2430	$54x^9$ Θ'=486	$54x^{45}$ Π'=2430	Π'/Θ'=5 Π'/Ω'=45 Θ'/Ω'=9
a=3 v=64 e=144	$9x^{16}$ CI=18432	$144x^{16}$ Θ'=2304	$144x^{128}$ Π'=18432	Π'/Θ'=8 Π'/Ω'=128 Θ'/Ω'=16
a=4 v=125 e=300	$12x^{25}$ CI=82500	$300x^{25}$ Θ'=7500	$300x^{275}$ Π'=82500	Π'/Θ'=11 Π'/Ω'=275 Θ'/Ω'=25

Table 9. Formulas for the three polynomials in some selected nets

(a) Cubic *pcu* net $C(a,b,c)_{net}$; (Figure 2b); (G_{cut} isometric to G)

$v(C(a,a,a)_{net})=(a+1)^3$; $c(C(a,a,a)_{net}=c=(a+1)^2$; $m(C(a,a,a)_{net}=m=3a$

$$\Omega(C(a,a,a),x)=m\cdot x^c=3a\cdot x^{(a+1)^2}$$

$$\Theta(C(a,a,a),x)=mc\cdot x^c=3a(a+1)^2\cdot x^{(a+1)^2}$$

$$\Pi(C(a,a,a),x)=mc\cdot x^{c(m-1)}=3a(a+1)^2\cdot x^{(a+1)^2(3a-1)}$$

$$\frac{\Pi'}{\Theta'}=\frac{mc(e-c)}{mc^2}=\frac{e}{c}-1=m-1;\ \frac{\Pi'}{\Omega'}=\frac{mc(e-c)}{mc}=e-c;\ \frac{\Theta'}{\Omega'}=\frac{mc^2}{mc}=c$$

$$\Omega(C(a,b,c),x)=a\cdot x^{(b+1)(c+1)}+b\cdot x^{(a+1)(c+1)}+c\cdot x^{(a+1)(b+1)}$$

$$\Omega(C(a,a,c),x)=2a\cdot x^{(a+1)(c+1)}+c\cdot x^{(a+1)^2}$$

$$\Omega(C(a,a,a),x)=3a\cdot x^{(a+1)^2}$$

Table 9. (continued)

(b) *Med*(C(a,b,c) $_{\text{net}}$); (Figure 3a)
$\Omega(Med(\mathrm{C})(a,b,c),x) = 4(a+1)\cdot\sum_{i=1}^{\min(b,c)-1} x^{2i} + 2(\lvert b-c\rvert+1)(a+1)\cdot x^{2\min(b,c)} +$ $4(b+1)\cdot\sum_{i=1}^{\min(a,c)-1} x^{2i} + 2(\lvert a-c\rvert+1)(b+1)\cdot x^{2\min(a,c)} +$ $4(c+1)\cdot\sum_{i=1}^{\min(a,b)-1} x^{2i} + 2(\lvert a-b\rvert+1)(c+1)\cdot x^{2\min(a,b)}$
$\Omega(Med(\mathrm{C})(a,a,c),x) = 8(a+1)\cdot\sum_{i=1}^{\min(a,c)-1} x^{2i} + 4(\lvert a-c\rvert+1)(a+1)\cdot x^{2\min(a,c)} + 4(c+1)\cdot\sum_{i=1}^{a-1} x^{2i} + 2(c+1)\cdot x^{2a}$
$\Omega(Med(\mathrm{C})(a,a,a),x) = 12(a+1)\cdot\sum_{i=1}^{a-1} x^{2i} + 6(a+1)\cdot x^{2a} = 6(a+1)[2\sum_{i=1}^{a-1} x^{2i} + x^{2a}]$
(c) *Med*(*Med*(OP))CO$_{\mathbf{60}}$(a,b,c)$_{\text{net}}$; (Figure 3b)
$\Omega(\mathrm{CO}_{60}(a,b,c),x) = 8(a+b+c)\cdot x^2 + (16(ab+ac+bc)-12(a+b+c))\cdot x^3 +$ $+((12abc+2(a+b+c))\cdot x^4 + ((12abc-6(ab+ac+bc)+2(a+b+c))\cdot x^6$
$\Omega(\mathrm{CO}_{60}(a,a,c),x) = 8(2a+c)\cdot x^2 + (16(a^2+2ac)-12(2a+c))\cdot x^3 + ((12a^2c+2(2a+c))\cdot x^4 +$ $+((12a^2c-6(a^2+2ac)+2(2a+c))\cdot x^6$
$\Omega(\mathrm{CO}_{60}(a,a,a),x) = 6a(4\cdot x^2 + (8a-6)\cdot x^3 + (2a^2+1)\cdot x^4 + (2a^2-3a+1)\cdot x^6)$

Conclusions

Three counting polynomials: Omega Ω, Equidistance Θ and Non-Equidistance Π have been defined and their mutual inter-relations established. All the three polynomials count sets of edges related to *quasi-orthogonal cut "qoc"* strips, at their turn related to partial cubes.

It was shown that the indices *CI* (derived from Omega polynomial) and *PI* (derived from Π polynomial) show identical values if all the subgraphs G_{cut} (obtained by cutting-off the two edges searched for equidistance) are isometric to *G*. Examples of graphs showing $CI = PI$ and $CI \neq PI$, respectively, were presented.

Extension from faces to rings (namely *strong rings*, which are not the sum of other smaller rings) enabled calculation of $\Omega(G,x)$ in 3D networks, either bipartite or non-bipartite. Analytical close formulas for the polyhex graphs of acenes and phenacenes, and for some cubic lattices and their corresponding cages were derived.

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