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Dedicated to Professor Mircea Diudea on the Occasion of His 65th Anniversary

TOPOLOGICAL INDICES IN HYPERTUBES OF HYPERCUBES

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ABSTRACT. A topological index is a single number descriptor that characterizes the molecular graph topology up to isomorphism. Hyper-tubes, open or closed, consisting of hyper-cubes of *n*-dimensions have been designed and formulas for some topological indices, counting vary substructures or characteristics, were established.

Keywords: *graph, topological index, n-cube, hyper-tube, hyper-torus, n-dimensional space*

INTRODUCTION

Schläfli [1] was the first scientist that described spaces of dimension higher than three, namely the six regular 4D-polytopes, also called polychora. These are as follows: 5-Cell {3,3,3}; 8-Cell {4,3,3}; 16-Cell {3,3,4}; 24-Cell {3,4,3}; 120-Cell {5,3,3} and 600-Cell {3,3,5}. Five of them can be associated to the Platonic solids but the sixth one, the 24-cell has no a 3D equivalent; it consists of 24 octahedral cells, 6 cells meeting at each vertex.Among the four dimensional polytopes, 5-Cell and 24-Cell are self-dual while the others are pairs: (8-Cell & 16-Cell); (120-Cell & 600-Cell). In the above, {*p*, *q*, *r*} are the Schläfli symbols: the symbol {*p*} denotes a regular polygon for integer *p*, or a

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star polygon for rational *p*; the symbol {*p*, *q*} denotes a 3D-object tessellated by *p*-gons while *q* is the vertex-figure (*i.e.*, the number of *p*-gons surrounding each vertex); the symbol {*p*, *q*, *r*} describes a 4D-structure, in which *r* 3D-objects join at any edge (*r* being the edge-figure) of the polytope, and so on. The Schläfli symbol has the nice property that its reversal gives the symbol of the dual polytope.

In dimensions 5 and higher, there are only three kinds of convex regular polytopes; no non-convex regular polytopes exist [2-4]. In the following, some details are given.

The ***n-simplex*** [2] has theSchläfli symbol $\{3^{n-1}\}$, and the number of its *k*-faces is given by the combinatorial formula $\binom{n+1}{k+1}$; it is a generalization of the triangle or tetrahedron to any dimensions.For example, a 0-simplex is a point, a 1-simplex is a line segment, a 2-simplex is a triangle, a 3-simplex is the tetrahedron, and a 4-simplex is the 5-cell.

The ***hypercube*** [2] is a generalization of the 3-cube to *n*-dimensions and is also called an *n*-Cube Q_n. It is a regular polytope with mutually perpendicular sides, thus being an orthotope. Its Schläfli symbol is $\{4,3^{n-2}\}$ and *k*-facesare counted by the formula $2^{n-k}\binom{n}{k}$.The hypercube can also be expressed as the Cartesian product of the complete graph K_2: $Q_n = \square_{i=1}^{n} K_2$.

The ***n-orthoplex* or cross-polytope** [2] has the Schläfli symbol $\{3^{n-2},4\}$ and its *k*-faces are counted by the formula $2^{k+1}\binom{n}{k+1}$; it is the dual of Q_n, in any *n*-dimensions. The facets of a cross-polytope are simplexes of the previous dimensions, while its vertex figures are other cross-polytopes of lower dimensions.

To investigate an *n*-dimensional polytope, a formula, due to Euler [5] (see also Schläfli [1]) is used:

$$\sum_{i=0}^{n-1}(-1)^i f_i = 1-(-1)^n \tag{1}$$

For *n*=3, eq (1) reduces to the simpler (well-known) Euler relation

$$v-e+f=2(1-g) \tag{2}$$

with *v*, *e*, *f* and *g* being the vertices, edges, 2-faces and the genus, respectively; *g*=0 for the sphere and *g*=1 for the torus.

It was conjectured by Diudea [6, 7] that the alternating sum for objects embedded in surfaces other than the sphere accounts for the genus of the embedding surface:

$$\sum_{k=0}^{n}(-1)^k f_k = \chi(M) = 2(1-g); n>1; k=0,1,..n. \tag{3}$$

It means that summation by (1) gives 2 and zero (for odd and even dimension, respectively) because the embedding surface was the sphere (see also (2)). In tori, with g=1, χ=0 irrespective of the dimension of the embedded structure.

HYPERCUBES IN HIGH-DIMENSIONAL TUBULAR STRUCTURES

It is well-known [2] that the number of k-cubes $Q_n(k)$ contained in the hypercube Q_n can be calculated by

$$Q_n(k) = 2^{n-k}\binom{n}{k}; \qquad k = 0,..,n-1 \tag{4}$$

Hypercube (Figure 1) is isomorphic to the Hässe diagram of a finite Boolean algebra [2].

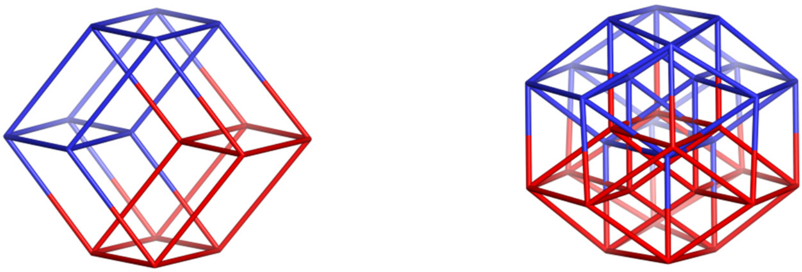

Figure 1. Hypercubes: the Tesseract or Q_4.16 hypercube (left) and Q_5.32 hypercube (right).

Open Tubes

In a recent paper [8], Moldovan and Diudea proposed the embedding of n-Cube in surfaces other than the sphere (Figures 2 and 3).

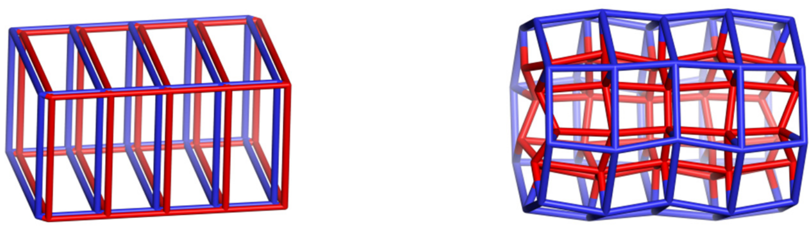

Figure 2. A hyper-tube TU(4,5),Q_4.40 (left) and a hyper-tube TU((4,8,5),Q_3.80 (right)

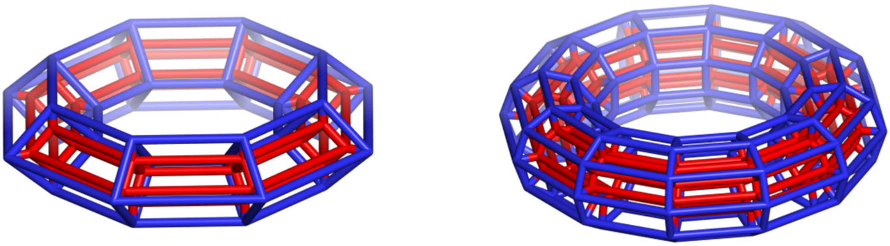

Figure 3. An elementary double-wall torus T((4,8), Q_4.64, of square section (left) and T((4,9,12),Q_3.216, with octagonal section and 16 units T((4,9,1),Q_3.36 (right)

The *k*-dimensional substructures of a simple hyper-tube TU((4,*r*),Q_n) (Figure 2, left) are counted from the hypercube $Q_n(k)$ substructures by formulas:

$$f_r = (r/2-1)/n \qquad f_k = (r/2)+k\cdot f_r \qquad k=0,1,..,n-1 \tag{5}$$
$$TU((4,r),Q_n,k) = Q_n(k)\cdot f_k\,;\;\; TU((4,r),Q_n,(k+1)) = r$$

From Table 1, one can see that the alternation sum of figures (equaling the value of χ) gives: zero for even dimension and 2 for the even dimension "Dim" of the hyper-tube. It means that the elementary hyper-tube TU((4,*r*),Q_n,) is like the sphere (*i.e.*, both having the genus *g*=0).

Table 1. Figure count in two hyper-tubes embedding hyper-cubes

Structure \ *k*	0	1	2	3	4	5	6	χ	Dim
TU((4,5),Q_5).80	80	224	248	136	37	5	-	0	6
Q_5	32	80	80	40	10	0	-	2	5
f_k	2.5	2.8	3.1	3.4	3.7	4	-	-	-
$Q_5 \times f_k$ & *r*	80	224	248	136	37	5	-	0	6
TU((4,5), Q_6).160	160	528	720	520	210	45	5	2	7
Q_6	64	192	240	160	60	12	-	0	6
f_k	2.5	2.75	3	3.25	3.5	3.75	4	-	-
$Q_6 \times f_k$ & *r*	160	528	720	520	210	45	5	2	7

In a more complex hyper-tube(Figure 2, right), each unit in the tube TU((4,*r*,*s*),Q_n) is an elementary hyper-torus T((4,*r*),Q_n) (Figure 3, left) while there are *s*-units along the tube.

The *k*-dimensional substructures of a complex hyper-tube TU((4,*r*,*s*),Q_n) are counted from the previous dimensional substructures of the elementary hyper-torus T((4,*r*),Q_n), by formulas:

$$TU((4,r,1),Q_n,k)) = T((4,r),Q_{n\text{-}1},k) + T((4,r),Q_{n\text{-}1},(k-1)) \qquad (6)$$

$$TU((4,r,s),Q_n,k) = s \times TU((4,r,1),Q_n,k)) + T((4,r),Q_{n\text{-}1},k); \qquad (7)$$
$$k = 0,1,..,n-1; n > 3$$

Table 2 gives details of the calculation of substructures in case of the hyper-tube TU((4,9,7),Q_5).504.Formulas work for any integer *n*>3.

Table 2. Figure countin the hyper-tubeTU((4,9,7),Q_5).504

Structure \ *k*	0	1	2	3	4	5	χ	Dim
TU((4,9,7),Q_5).504	504	1692	2214	1413	441	54	0	6
T((4,9),Q_4).72	72	180	162	63	9	-	0	5
-	-	72	180	162	63	9	-	-
TU((4,9,1),Q_5).72	72	252	342	225	72	9	0	6
TU((4,9,1),Q_5)×6	432	1512	2052	1350	432	54	-	-
+ T((4,9),Q_4).72	72	180	162	63	9	0	-	-
Sum	504	1692	2214	1413	441	54	0	6

Tori

When the end-faces of a hypertube are identified, it results in a closed hyper-tube or a hyper-torus (Figure 3). We studied particularly the tori T(4,*r*) and T(4,*r*,*s*), according to Diudea's discretization procedure [9].

The *k*-dimensional substructures of a simple hyper-torus T((4,*r*),Q_n) (Figure 3, left) are counted on the basis of the hypercube $Q_n(k)$ substructures by the following formulas:

$$f_r = (r/2)/n \qquad f_k = (r/2) + k \cdot f_r \qquad k = 0,1,..,n-1 \qquad (8)$$
$$T((4,r),Q_n,k) = Q_n(k) \cdot f_k; \qquad T((4,r),Q_n,(k+1)) = r$$

Formulas can be easily verified from data listed in Table 3. The hyper-torusT((4,*r*),Q_n,*k*) is herein named "elementary" because it is a constituent of the more complex hyper-tubes and hyper-tori built up on the ground of hyper-cubes.

Table 3. Figure count for the hyper-torus T((4,8),Q_n)

Torus \ *k*	0	1	2	3	4	5	6	7	f_r	Deg(*v*)	χ
Q_3	8	12	6	0	0	0	0	0	0	3	2
Q_4	16	32	24	8	0	0	0	0	0	4	0
Q_5	32	80	80	40	10	0	0	0	0	5	2
Q_6	64	192	240	160	60	12	0	0	0	6	0
Q_3T_4	32	64	40	8	0	0	0	0	4/3	4	0
Q_4T_5	64	160	144	56	8	0	0	0	4/4	5	0
Q_5T_6	128	384	448	256	72	8	0	0	4/6	6	0
Q_6T_7	256	896	1280	960	400	88	8	0	4/6	7	0

The number of rings *R* around any point in the hyper-torus is given by formula

$$R(T((4,r),Q_n)) = 4^{(n-1)(n+2)/2} \tag{9}$$

The vertex degree in the hyper-torus T((4,*r*),Q_n) equals (*n*+1). The torus is vertex transitive but its edges f_1 and faces f_2 are split in two equivalence classes.

In a more complex hyper-torus (see Figure 3, right); each unit T((4,*r*,1),Q_n) in the torus T((4,*r*,*s*),Q_n) is an elementary hyper-torus T((4,*r*),Q_n) while there are *s*-units around the central hollow.

The *k*-faces of a hyper-torus T((4,*r*,*s*),Q_n) are counted from the previous dimensional substructures of the elementary hyper-torus T((4,*r*),Q_n), by formulas:

$$T((4,r,1),Q_n,k) = T((4,r),Q_{n-1},k) + T((4,r),Q_{n-1},(k-1)) \tag{10}$$

$$T((4,r,s),Q_n,k) = s \times T((4,r,1),Q_n,k)\,;\, k = 0,1,..,n-1; n > 3 \tag{11}$$

Details are given in Table 4; formulas work for any integer *n*>3.

Table 4. Figure count in the hyper-torus T((4,8,16),Q_7).4096

Structure \ *k*	0	1	2	3	4	5	6	7	χ
T((4,8),Q_6).256	256	896	1280	960	400	88	8	0	0
	-	256	896	1280	960	400	88	8	-
T((4,8,1),Q_7).256	256	1152	2176	2240	1360	488	96	8	0
T((4,8,16),Q_7).4096	4096	18432	34816	35840	21760	7808	1536	128	0

The vertex degree in the hyper-torus T((4,*r*,*s*),Q_n) equals (*n*+2). This torus is vertex transitive but its edges f_1 and faces f_2 are split in three equivalence classes.

Note the difference between the hyper-cube and TU((4,*r*),Q_n) on one hand and the hyper-tube TU(4,*r*,*s*),Q_n), on the other hand: the figure sum gives alternating 0 and 2 for the hyper-cube, at even and odd *n*-dimension, respectively (Table 3), while the last structures provide zero, irrespective of *n* parity. This is because torus has the genus *g*=1 [10].

OMEGA POLYNOMIAL AND CI INDEX

A counting polynomial [11] is a representation of a graph *G*(*V*,*E*), with the exponent *a* showing the extent of partitions *p*(*G*), $\cup p(G) = P(G)$ of a graph property *P*(*G*) while the coefficient $p(a)$ is related to the number of partitions of extent *a*.

$$P(x) = \sum_a p(a) \cdot x^a \tag{12}$$

Let *G* be a connected graph, with *V*(*G*) and *E*(*G*) being the vertex set and edge set, respectively. Two edges *e*=(*u*,*v*) and *f*=(*x*,y) of *G* are *codistant* (briefly: *e co f*) if they fulfill the relation [12]

$$d(v,x) = d(v,y) + 1 = d(u,x) + 1 = d(u,y) \tag{13}$$

where *d* is the shortest-path distance function. The relation *co* is reflexive (*e co e*) and symmetric (*e co f*) for any edge *e* of *G* butis not necessarily transitive. A graph is called a *co-graph* if the relation *co* is also transitive and thus *co* is an equivalence relation.

Let $C(e) := \{f \in E(G); f\ co\ e\}$ be the set of edges in *G*, codistant to $e \in E(G)$. The set *C*(*e*) is provided by an orthogonal edge-cutting procedure: take a straight line segment, orthogonal to the edge *e*, and intersect it and all other edges (of a polygonal plane graph) parallel to *e*. The set of these intersections is called an *orthogonal cut* of *G*, with respect to *e*. If *G* is a *co-graph* then its orthogonal cuts $C_1, C_2, ..., C_k$ form a partition of *E*(*G*):

$$E(G) = C_1 \cup C_2 \cup ... \cup C_k,\ C_i \cap C_j = \varnothing, i \neq j \tag{14}$$

A subgraph *H*⊆*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*. The relation *co* is related to Djoković ~ [13] and Winkler Θ [14] relations (see also [15]).

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*. Then *e co f* holds by the assumption that faces are isometric. The relation *co* is defined in the whole graph while *op* is defined only in faces/rings. Relation *op* will partition the edges set of *G* into *opposite* edge *strips ops*, as follows. (i) Any two subsequent edges of an *ops* are in *op* relation; (ii) Any three subsequent edges of such a strip belong to adjacent faces; (iii) In a plane graph, the inner dual of an *ops* is a path (however, in 3D networks, the ring/face interchanging will provide *ops* which are no more paths); (iv) The *ops* is taken as maximum possible, irrespective of the starting edge. The choice about the maximum size of face/ring, and the face/ring mode counting, will decide the length of the strip. Note that *ops* are *qoc* (quasi orthogonal cuts), meaning the transitivity relation is, in general, not obeyed.

The Omega polynomial $\Omega(x)$ [16-18] is defined on the ground of opposite edge strips *ops* $S_1, S_2, ..., S_k$ in the graph. Denoting by *m* the number of *ops* of cardinality/length *s*=|*S*|, we can write

$$\Omega(x) = \sum_s m \cdot x^s \tag{15}$$

The first derivative (in *x*=1) can be taken as a graph invariant or a topological index:

$$\Omega'(1) = \sum_s m \cdot s = |E(G)| \tag{16}$$

An index, called Cluj-Ilmenau *CI*(*G*) [12], was defined on $\Omega(x)$:

$$CI(G) = \{[\Omega'(1)]^2 - [\Omega'(1) + \Omega''(1)]\} \tag{17}$$

In tree graphs, the Omega polynomial counts the non-opposite edges, all being included in the term of exponent *s*=1. Omega polynomial was thought to describe the covering of polyhedral nano-structures or the tiling of crystal-like lattices, as a complementary description of the crystallographic one.

In *n*-dimensional space, Omega polynomial could be useful in topological characterization of structures in which formulas for *k*-substructures are not known, the polynomial being more easily to count.

The following tables provide analytical formulas for the hyper-cubes (Tables 5 and 6), hyper-tubes (Tables 7 to 10) and hyper-tori (Tables 11 to 14) and numerical examples as well.

Table 5. Formulas for Omega polynomial in hyper-cubes Q_n

1	$\Omega(Q_n, x) = n \cdot x^{2^{n-1}}$
2	$\Omega'(1) = e(Q_n) = \lvert E(Q_n)\rvert = n \cdot 2^{n-1}$
3	$\Omega''(1) = n \cdot 2^{n-1} \cdot (2^{(n-1)} - 1)$
4	$CI(T((4,r),Q_n)) = n(n-1) \cdot 4^{n-1}$

Table 6. Omega polynomial in hyper-cubes Q*n*; examples

Vertices	Edges	Q*n*	Deg(*v*)	Omega polynomial	CI
16	32	4	4	4X^8	768
32	80	5	5	5X^16	5120
64	192	6	6	6X^32	30720

Table 7. Formulas for Omega polynomial in hyper-tubes ((4,*r*),Q*n*)

1	$\Omega(TU((4,r),Q_n),x) = (r-1)\cdot x^{4\cdot 2^{n-3}} + (n-1)\cdot x^{2r\cdot 2^{n-3}}$
2	$\Omega'(1) = e(TU((4,r),Q_n)) = 2^{n-3}\cdot(2r+2rn-4)$
3	$v(TU((4,r),Q_n)) = 4r\cdot 2^{n-3}$
4	$\Omega''(1) = 2^{n-4}(4r-4\cdot 2^n\cdot r+4\cdot 2^n+2^n\cdot r^2+4nr-2^n\cdot nr^2-8)$
5	$CI(TU((4,r),Q_n)) = 4^{n-2}(n^2r^2+nr^2-4nr+2r^2-8r+8)$

Table 8. Omega polynomial in TU((4,*r*),Q*n*)

Structure	Vertices	Edges	Q*n*	Omega polynomial	CI
TU(4,5)	20	36	3	4X^4+2X^10	1032
	40	92	4	4X^8+3X^20	7008
	80	224	5	4X^16+4X^40	42752
TU(4,6)	24	44	3	5X^4+2X^12	1568
	48	112	4	5X^8+3X^24	10496
	96	272	5	5X^16+4X^48	63488

Table 9. Formulas for Omega polynomial in hyper-tubes TU((4,*r*,*s*), Q*n*)

1	$\Omega(TU((4,r,s),Q_n),x) = r\cdot x^{2s\cdot 2^{n-3}} + (s-1)\cdot x^{2r\cdot 2^{n-3}} + (n-2)\cdot x^{rs\cdot 2^{n-3}}$
2	$\Omega'(1) = e(TU((4,r,s),Q_n)) = 2^{n-3}\cdot(2rs-2r+nrs)$
3	$v(TU((4,r,s),Q_n)) = 2rs\cdot 2^{n-3}$
4	$\Omega''(1) = 2^{n-6}\cdot r\cdot(16s+4\cdot 2^n\cdot r-4\cdot 2^n\cdot s^2+8\cdot n\cdot s+2\cdot 2^n\cdot r\cdot s^2-4\cdot 2^n\cdot r\cdot s-2^n\cdot n\cdot r\cdot s^2-16)$
5	$CI(TU((4,r,s),Q_n)) = 4^{n-3}\cdot r\cdot(8r+6r\cdot s^2-4s^2-12r\cdot s+n^2\cdot r\cdot s^2-4n\cdot r\cdot s+3n\cdot r\cdot s^2)$

Table 10. Omega polynomial in TU((4,*r*,*s*),Q*n*)

Structure	Vertices	Edges	Q*n*	Omega polynomial	*r*	*s*	CI
TU(5,5)	50	115	3	5X^10+4X^10+1X^25	5	5	11700
	100	280	4	5X^20+4X^20+2X^50	5	5	69800
	200	660	5	5X^40+4X^40+3X^100	5	5	391200
TU(9,7)	126	297	3	9X^14+6X^18+1X^63	9	7	80532
	252	720	4	9X^28+6X^36+2X^126	9	7	471816
	504	1692	5	9X^56+6X^72+3X^252	9	7	2613024

Table 11. Formulas for Omega polynomial in hyper-tori T((4,*r*), Q*n*

1	$\Omega(T((4,r),Q_n),x) = r\cdot x^{(2^{n-1})} + (n-1)\cdot x^{(r\cdot 2^{n-2})}$
2	$\Omega'(1) = e(T((4,r),Q_n)) = r(n+1)\cdot 2^{n-2}$
3	$v(T((4,r),Q_n)) = r\cdot 2^{n-1}$
4	$\Omega''(1) = (-)r\cdot 2^{n-4}(4n + r\cdot 2^n - 2^{n+2} - r\cdot n\cdot 2^n + 4)$
5	$CI(T((4,r),Q_n)) = r\cdot 4^{n-2}(r\cdot n^2 + r\cdot n + 2r - 4)$

Table 12. Omega polynomial in hyper-tori T((4,*r*), Q*n*); examples

Vertices	Edges	Q*n*	Deg(*v*)	Omega polynomial	CI
T(4,8)					
32	64	3	4	8X^4+2X^16	3456
64	160	4	5	8X^8+3X^32	22016
128	384	5	6	8X^16+4X^64	129024
T(4,9)					
288	1008	6	7	9X^32+5X^144	903168
576	2304	7	8	9X^64+6X^288	4773888
1152	5184	8	9	9X^128+7X^576	24403968

Table 13. Formulas for Omega polynomial in hyper-tori T((4,*r*,*s*), Q*n*)

1	$\Omega(T((4,r,s),Q_n),x) = s\cdot x^{r\cdot 2^{n-2}} + r\cdot x^{s\cdot 2^{n-2}} + (n-2)\cdot x^{rs\cdot 2^{n-3}}$
2	$\Omega'(1) = e(T((4,r,s),Q_n)) = rs(n+2)\cdot 2^{n-3}$
3	$v(T((4,r,s),Q_n)) = rs\cdot 2^{n-2}$
4	$\Omega''(1) = (-)2^{n-6}rs(8n - 2^{n+2}r - 2^{n+2}s + 2^{n+1}rs - 2^n nrs + 16)$
5	$CI(T((4,r,s)Q_n)) = 2^{2(n-3)}rs(rsn^2 + 3rsn - 4r - 4s + 6rs)$

Table 14. Omega polynomial in hyper-tori T((4,*r*,*s*), Q*n*); examples

Vertices	Edges	Q*n*	Deg(*v*)	Omega polynomial	CI
T(4,5,15)					
150	375	3	5	15X^10+5X^30+1X^75	129000
300	900	4	6	15X^20+5X^60+2X^150	741000
600	2100	5	7	15X^40+5X^120+3X^300	4044000
T(4,8,8)					
128	320	3	5	16X^16+1X^64	94208
256	768	4	6	16X^32+2X^128	540672
512	1792	5	7	16X^64+3X^256	2949120

CLUJ POLYNOMIAL AND RELATERD INDICES

In bipartite graphs, the coefficients of *CJ* polynomial [19,20] can be calculated by an orthogonal edge-cut procedure [20,21]. In this respect, a more theoretical background is needed.

A graph *G* is a *partial cube* if it is embeddable in the hypercube C(n). For any edge *e*=(*u*,*v*) of a connected graph *G* let n_{uv} denote the set of vertices lying closer to *u* than to *v*: $n_{uv} = \{ w \in V(G) \mid d(w,u) < d(w,v) \}$. It follows that $n_{uv} = \{ w \in V(G) \mid d(w,v) = d(w,u) + 1 \}$. The sets (and subgraphs) induced by these vertices, n_{uv} and n_{vu}, are called *semicubes* of *G*; the semicubes are called *opposite semicubes* and are disjoint [22,23]. A graph *G* is bipartite if and only if, for any edge of *G*, the opposite semicubes define a partition of *G*: $n_{uv} + n_{vu} = v = |V(G)|$. These semicubes are just the vertex proximities of (the endpoints of) edge *e*=(*u*,*v*), which CJ_e polynomial counts. In partial cubes, the semicubes can be estimated by an orthogonal edge-cutting procedure.

Function of the mathematic operation, three polynomials can be written with these semicubes:

(i) *Cluj-Sum*, symbolized *CJS* (obtained by summation) [24-26]:

$$CJS(x) = \sum_{e} \left(x^{v_k} + x^{v - v_k} \right) \tag{18}$$

(ii) PI_v (vertex, Padmakar−Ivan index [27]) polynomial (obtained by pairwise summation) [28-30]

$$PI_v(x) = \sum_{e} x^{v_k + (v - v_k)} \tag{19}$$

(iii) *Cluj-Product*, symbolized *CJP* (obtained by pairwise product). [19,20,26,32]. It was also named *Szeged* polynomial *SZv* [29,30,33]:

$$CJP(x) = SZ_v(x) = \sum_{e} x^{v_k (v - v_k)} \tag{20}$$

In hypercubes, the formulas for calculating the Cluj-related polynomials and derived topological indices (as the first derivative, in *x*=1) are given in Table 15 while examples are provided in Tables 16 to 18. Observe that the first derivative of CJs and PI_v are the same (Tables 16 and 17) but the second derivative (in *x*=1) is however, different.

Table 15. Formulas for Cluj and PI_v polynomial in hyper-cubes

	Formulas
1	$v(Q_n)=\|V(Q_n)\|=2^n$; $e(Q_n)=\|E(Q_n)\|=n\cdot 2^{n-1}$
2	$CJS(Q_n,x)=n(v/2)x^{v/2}+n(v/2)x^{v/2}=n(2^{n-1})\cdot x^{2^{n-1}}+n(2^{n-1})\cdot x^{2^{n-1}}=n\cdot 2^n\cdot x^{2^{n-1}}$
3	$CJS'(1)=n\cdot 2^{2n-1}$
4	$CJS''(1)=n\cdot 2^{2(n-1)}\cdot(2^n-2)$
5	$PI_v(Q_n,x)=ex^v=n\cdot 2^{n-1}\cdot x^{2^n}$
6	$PI_v'(1)=n\cdot 2^{2n-1}$
7	$PI_v''(1)=n\cdot 2^{2n-1}\cdot(2^n-1)$
8	$CJP(Q_n,x)=n(v/2)x^{(v/2)(v/2)}=n\cdot 2^{n-1}\cdot x^{2^{2(n-1)}}$
9	$CJP'(1)=n\cdot 2^{n-1}\cdot 2^{2(n-1)}=SZ_v$

Table 16. Cluj polynomial CJS in hypercube Q_n

Q_n : n	CJS(x)	CJS'	CJS"
3	12x^4+12x^4	96	288
4	32x^8+32x^8	512	3584
5	80x^16+80x^16	2560	38400
6	192x^32+192x^32	12288	380928

Table 17. PI_v polynomial in hypercube Q_n

Q_n : n	PIv(x)	PIv'	PIv"
3	12x^8	96	672
4	32x^16	512	7680
5	80x^32	2560	79360
6	192x^64	12288	774144

Table 18. Cluj polynomial CJP in hypercube Q_n

Q_n : n	CJP(x)	CJP'=SZ_v
3	12x^(4*4)	192
4	32x^(8*8)	2048
5	80x^(16*16)	20480
6	192x^(32*32)	196608

COMPUTATIONAL DETAILS

The design and properties of the studied structures was performed by our original Nano Studio [34] software program.

The numerical data resulted in calculation of polynomials and related topological indices appeared as integer sequences. To find the corresponding analytical formulas, we made use of OEIS, "The On-Line Encyclopedia of Integer Sequences" [35].

CONCLUSIONS

In this paper, several polynomials and the corresponding topological indices have been computed for tubular and toroidal hyper-structures made from hyper-cube units. Analytical formulas were established and numerical examples given.

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