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Omega polynomial in twisted (4,4) tori

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Abstract. Define quasi orthogonal cuts *qoc* with respect to a given edge in a graph $G=G(V,E)$ as the smallest subset of edges closed under taking opposite edges on faces. Omega polynomial $\Omega(G,x)$ is defined on the qoc strips of all extent in G. Analytical close formulas for calculating $\Omega(G,x)$ in twisted (4,4)S and (4,4)R tori are derived.

1. Counting Polynomials in Chemistry

A counting polynomial can be written in the form:

$$P(G,x) = \sum_k m(G,k) \cdot x^k \qquad (1)$$

can be regarded 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 number of partitions of extent k.

In the Mathematical Chemistry literature, the counting polynomials have first been introduced by Hosoya:[1,2] $Z(G,x)$ counts independent edge sets while $H(G,x)$ (initially called Wiener and later Hosoya)[3,4] counts the distances in G. Further, Hosoya proposed the sextet polynomial[5-8] for counting the resonant rings in a benzenoid molecule.[9,10] Other counting polynomials have later been proposed: *independence*[11-13] *king*, *color*, *star* or *clique polynomials*.[14-18] More about polynomials the reader can find in ref 19.

The aim of this paper is to find close analytical relations for Omega polynomial in some twisted (4,4) tori .

2. Definitions

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

$$d(x,v) = d(x,u) + 1 = d(y,v) + 1 = d(y,u) \qquad (2)$$

For some edges of a connected graph G there are the following relations satisfied:[20]

$$e\ co\ e \qquad (3)$$

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

$$e\ co\ f\ \&\ f\ co\ h \Rightarrow e\ co\ h \qquad (5)$$

though the relation (5) 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., $C(e)$ obeys (3) to (5)), 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 $Ci \cap Cj = Ø$ for $i \neq j, i, j = 1,2,..,k$.

Let $G(V,E)$ be a connected graph and d be its distance function. A subgraph $H \subseteq G$ is called *isometric*, if $d_H(u,v) = d_G(u,v)$ $\in$; it is *convex* if any shortest path in G between vertices of H belongs to H. A *partial cube* is an isometric subgraph of a *hypercube* Q_n; this can be obtained as a Cartesian product $Q_n = \Box_{i=1}^{n} K_2$. Examples of partial cubes are even cycles, benzenoid graphs, phenylenes, trees, etc.[21,22]

A *graph G is a co-graph if and only if it is a partial cube.* A *quasi-orthogonal cut qoc* with respect to a given edge is the smallest subset of edges closed under taking opposite edges on faces. Since the transitivity relation (5) of the *co* relation is not necessarily obeyed, *qoc* represents a new concept within the cut methods. Any *oc* strip is a *qoc* strip but the reverse is not always true.[23,24]

3. Omega Polynomial

Let $m(G,c)$ be the number of *qoc* strips of length c (*i.e.*, the number of cut-off edges). The Omega polynomial is defined,[25] on the ground of *qoc* strips:

$$\Omega(G,x) = \sum_c m(G,c) \cdot x^c \qquad (6)$$

In a counting polynomial, the *first derivative* (in x=1) defines the type of the counted property:

$$\Omega'(G,1) = \sum_c m(G,c) \cdot c = e = |E(G)| \quad (7)$$

The Cluj-Ilmenau[20] index, $CI=CI(G)$, is calculable on Omega polynomial, as:

$$CI(G) = \{[\Omega'(G,1)]^2 - [\Omega'(G,1) + \Omega''(G,1)]\} \quad (8)$$

Figure 1 gives an example of calculation.

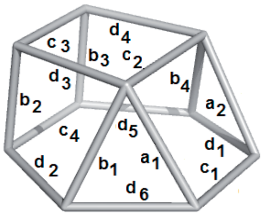

Figure 1. Omega polynomial in the graph G_1:
$\Omega(G,x) = x^2 + 2 \cdot x^4 + x^6$; $\Omega'(G,1) = 16 = e$; $CI = 184$

In tree graphs, the Omega polynomial simply counts the non-opposite edges, being included in the term of exponent c=1. 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. Indices derived from Omega polynomial are useful in describing the topology and predicting properties of nanostructures. [26]

4. Omega Polynomial in Twisted (4,4) Tori

The embedding of the square (4,4)S net on the torus (Figure 2a and 2c) can be made by circulating a c-fold cycle, circumscribed to the toroidal tube cross-section, around the large hollow of the torus. The subsequent *n images* of c-fold cycle, equally spaced are joined with edges, point by point, to form a polyhedral torus tiled by a tetragonal pattern. In all, $c \times n$ points are generated.[27-29] The (4,4)S covering can also be generated by the Cartesian product $C_c \square C_n$.[21]

The primary (4,4)S net can be changed to the rhombic (4,4)R pattern (Figure 2b and 2d) by the Medial Med operation on maps. The reader can consult recent papers[30-35] dealing with operations on maps.

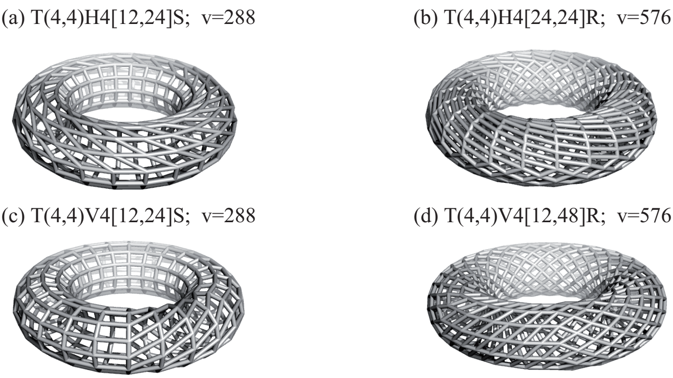

Figure 2. (4,4)S pattern (a and c) and (4,4)R pattern (b and d) embedded in the torus

Observe the (4,4)S net can be twisted either horizontally H or vertically V, thus resulting two isomeric embeddings, which are chiral. Accordingly, the medial transformed lattice, which shows the rhombic (4,4)R pattern, will also be twisted and chiral. The Med operation will double the number of points in the original object as:

$$Med(\mathrm{T(4,4)H}t[c,n]\mathrm{S}) \longrightarrow (\mathrm{T(4,4)H}t[2c,n]\mathrm{R}) \quad (9)$$

$$Med(\mathrm{T(4,4)V}t[c,n]S) \longrightarrow (\mathrm{T(4,4)V}t[c,2n]\mathrm{R}) \quad (10)$$

Table 1. Omega Polynomials in ((4,4) Tori: T(4,4)*t*[*c*,*n*]S

(1) H*t*; n=3c; *t* [12,36]

t	$\Omega(T,x)$	CI	Formula	Divisors
0	$36X^{12}+12X^{36}$	725760	$nx^{c}+tx^{cn/t}$	c /V*t*
1	$12X^{36}+1X^{432}$	544320	$cx^{n}+tx^{cn/t}$	c (**1**,5,7,11)
2	$12X^{36}+2X^{216}$	637632	$cx^{n}+tx^{cn/t}$	c (**2**,10)
3	$12X^{36}+3X^{144}$	668736	$cx^{n}+tx^{cn/t}$	c (**3**)
4	$12X^{36}+4X^{108}$	684288	$cx^{n}+tx^{cn/t}$	c (**4**,8)
6	$12X^{36}+6X^{72}$	699840	$cx^{n}+tx^{cn/t}$	c (**6**)
9	$12X^{36}+9X^{48}$	710208	$cx^{n}+tx^{cn/t}$	**n** (**9**)
12	$24X^{36}$	715392	$cx^{n}+tx^{cn/t}$	c,n (**12**)

(2) V*t*; n=3c; *t* [12,36]

t	$\Omega(T,x)$	CI	Formula	Divisors
0	$36X^{12}+12X^{36}$	725760	$nx^{c}+tx^{cn/t}$	c
1	$36X^{12}+1X^{432}$	554688		c (**1**,5,7,11)
2	$36X^{12}+2X^{216}$	648000		c (**2**,10)
3	$36X^{12}+3X^{144}$	679104		c (**3**,9)
4	$36X^{12}+4X^{108}$	694656		c (**4**,8)
6	$36X^{12}+6X^{72}$	710208		c (**6**)
12	$36X^{12}+12X^{36}$	725760		c (**12**)

The Omega polynomials were calculated by using Omega generator software[36] and the results, listed in Tables 1 and 2, are rationalised in Table 3 in terms of Diudea's symbolism for a toroidal network.[27,28]

Table 2. Omega Polynomials in ((4,4) Tori: Med(T(4,4)*t*[*c*,*n*]S)= T(4,4)*t*[*c*,*n*]R

(1) H*t*; n=2c; c = odd; *t* [**15**,30]

t	$\Omega(T,x)$	CI	Formula	Divisors
0	$30X^{60}$	3132000	$2tX^{2cn/t}$	c
1	$4X^{450}$	2430000	$4tX^{cn/t}$	c,n (**1**,7,11,13)
2	$2X^{900}$	1620000	$tX^{4cn/t}$	**n** (**2**,4,8,14)
3	$12X^{150}$	2970000	$4tX^{cn/t}$	c,n (**3**,9)
5	$20X^{90}$	3078000	$4tX^{cn/t}$	c,n (**5**)
6	$6X^{300}$	2700000	$tX^{4cn/t}$	**n** (**6**,12)
10	$10X^{180}$	2916000	$tX^{4cn/t}$	**n** (**10**)
15	$60X^{30}$	3186000	$4tX^{cn/t}$	c,n (**15**)

(2) H*t*; n=2c; c = even; not 2^k; *t* [**10**,20]

t	$\Omega(T,x)$	CI	Formula	Divisors
0	$20X^{40}$	608000	$2tX^{2cn/t}$	c
1	$2X^{400}$	320000	$2tX^{2cn/t}$	c (**1**,3,7,9)
2	$8X^{100}$	560000	$4tX^{cn/t}$	c,n (**2**,6)
4	$4X^{200}$	480000	$tX^{4cn/t}$	**n** (**4**,8)
5	$10X^{80}$	576000	$2tX^{2cn/t}$	c (**5**)
10	$40X^{20}$	624000	$4tX^{cn/t}$	c,n (**10**)

(3) H*t*; n=3c; c = even; not 2^k; r=3(odd); *t* [**10**,30]

t	$\Omega(T,x)$	CI	Formula	Divisors
0	$20X^{60}$	1368000	$2tX^{2cn/t}$	c
1	$3X^{200}+1X^{600}$	960000	$rtX^{2cn/rt}+ tX^{2cn/t}$	c,n (**1**,7)
2	$6X^{100}+2X^{300}$	1200000	$rtX^{2cn/rt}+ tX^{2cn/t}$	c,n (**2**,4,8)
3	$2X^{600}$	720000	$2t/rX^{2cnr/t}$	**n** (**3**,9)
5	$15X40+5X^{120}$	1344000	$rtX^{2cn/rt}+ tX^{2cn/t}$	c,n (**5**)
6	$4X^{300}$	1080000	$2t/rX^{2cnr/t}$	**n** (**6**)
10	$30X^{20}+10X^{60}$	1392000	$rtX^{2cn/rt}+ tX^{2cn/t}$	c,n (**10**)

(4) H*t*; n=4c; c = odd; r=4 (even)); *t* [**11**,44]

t	$\Omega(T,x)$	CI	Formula	Divisors
0	$22X^{88}$	3577728	$2tX^{2cn/t}$	c
1	$4X^{242}+2X^{484}$	3045328	$rtX^{2cn/rt}+2tX^{cn/t}$	c,n (**1**,3,5,7,9)
2	$2X^{968}$	1874048	$tX^{4cn/t}$	**n** (**2**,4,6,8,10)
11	$44X^{22}+22X^{44}$	3684208	$rtX^{2cn/rt}+2tX^{cn/t}$	c,n (**11**)

(5) H*t*; n=4c; c = even; not 2^k; r=4(even); *t* [**10**,40]

t	$\Omega(T,x)$	CI	Formula	Divisors
0	$20X^{80}$	2432000	$2tX^{2cn/t}$	c
1	$2X^{800}$	1280000	$2tX^{2cn/t}$	c (**1**,3,7,9)
2	$8X^{100}+4X^{200}$	2320000	$rtX^{2cn/rt}+2tX^{cn/t}$	c,n (**2**,6)
4	$4X^{400}$	1920000	tX^{cn}	**n** (**4**,8)
5	$10X^{160}$	2304000	$2tX^{2cn/t}$	c (**5**)
10	$40X^{20}+20X^{40}$	2512000	$rtX^{2cn/rt}+2tX^{cn/t}$	c,n (**10**)

(6) H*t*; n=2c; c = even =2^k; *t* [**16**,32]

t	$\Omega(T,x)$	CI	Formula	Divisors
0	$32X^{64}$	4063232	$2tX^{2cn/t}$	c
1	$2X^{1024}$	2097152	$2tX^{2cn/t}$	c (**1**,3,5,7,9,15)
2	$4X^{512}$	3145728	$2tX^{2cn/t}$	c (**2**,6,10,14)
4	$8X^{256}$	3670016	$2tX^{2cn/t}$	c (**4**,12)
8	$16X^{128}$	3932160	$2tX^{2cn/t}$	c (**8**)
16	$64X^{32}$	4128768	$4tX^{cn/t}$	c,n (**16**)

(7) H*t*=0/=V*t*=0/V*t*=*c*

t[c,n]	$\Omega(T,x)$	CI	Formula	Divisors
10[10,20]	$20X^{40}$	608000	$2tX^{2cn/t}$	c
10[10,30]	$20X^{60}$	1368000	$2tX^{2cn/t}$	c
10[10,40]	$20X^{80}$	2432000	$2tX^{2cn/t}$	c
11[11,44]	$22X^{88}$	3577728	$2tX^{2cn/t}$	c
15[15,30]	$30X^{60}$	3132000	$2tX^{2cn/t}$	c
16[16,32]	$32X^{64}$	4063232	$2tX^{2cn/t}$	c

(8) V*t*; $n = rc$; *t* [**9**,36]

t	$\Omega(T,x)$	CI	Formula	Divisors
0	$18X^{72}$	1586304	$2tX^{2cn/t}$	c
1	$2X^{648}$	839808	$2tX^{2cn/t}$	c (**1**,2,4,5,7,8)
3	$6X^{216}$	1399680	$2tX^{2cn/t}$	c (**3**,6)
9	$18X^{72}$	1586304	$2tX^{2cn/t}$	c (**9**)

Table 3. Omega Polynomial in Twisted (4,4)S/R Tori

T(4,4)S		
(1) H*t*; $n = rc$;	$\Omega(G,x) = c \cdot x^{n} + t \cdot x^{cn/t}$	$t = div\ c$ & $div\ n$
(2) V*t*; $n = rc$;	$\Omega(G,x) = n \cdot x^{c} + t \cdot x^{cn/t}$	$t = div\ c$ *t*=0; H=V; *t*=0=*c*
T(4,4)R		
(1) H*t* n=2c; c = odd	$\Omega(G,x) = 4t \cdot x^{cn/t}$ $\Omega(G,x) = t \cdot x^{4cn/t}$	$t = div\ c,n$ *t*=(*div n*)/2; *c* $t = div\ n$
(2) H*t* n=2c; c = even, not 2^k r=2	$\Omega(G,x) = 2t \cdot x^{2cn/t}$ $\Omega(G,x) = 4t \cdot x^{cn/t}$ $\Omega(G,x) = t \cdot x^{4cn/t}$	$t = div\ c$ $t = div\ c,n$ *t*=(*div n*)/2; *c* $t = div\ n$; not in case c=2^k
(3) H*t* n=3c; c = even, not 2^k r=3 (odd) r=3 (odd)	$\Omega(G,x) = 2t \cdot x^{2cn/t}$ $\Omega(G,x) = rt \cdot x^{2cn/rt} + t \cdot x^{2cn/t}$ $\Omega(G,x) = 2t/r \cdot x^{2cnr/t}$	$t = div\ c$ $t = div\ c,n$; *t*=*c* $t = div\ n$
(4) H*t* n=4c; c = odd; r=4 (even)	$\Omega(G,x) = rt \cdot x^{2cn/rt} + 2t \cdot x^{cn/t}$ $\Omega(G,x) = t \cdot x^{4cn/t}$	$t = div\ c,n$ *t*=(*div n*)/2; *c* $t = div\ n$
(5) H*t* n=4c; c = even, not 2^k r=4 (even) r=4 (even)	$\Omega(G,x) = 2t \cdot x^{2cn/t}$ $\Omega(G,x) = rt \cdot x^{2cn/rt} + 2t \cdot x^{cn/t}$ $\Omega(G,x) = t \cdot x^{4cn/t}$	$t = div\ c$ $t = div\ c,n$ *t*=(*div n*)/2; *c* $t = div\ n$
(6) H*t* n=2c; c = even=2^k	$\Omega(G,x) = 2t \cdot x^{2cn/t}$ $\Omega(G,x) = 4t \cdot x^{cn/t}$ not the case	$t = div\ c$ $t = div\ c,n$; *t*=*c* $t = div\ n$
(7) H*t*=0/=V*t*=0/V*t*=*c*	$\Omega(G,x) = 2t \cdot x^{2cn/t} = 2c \cdot x^{2n}$	
(8) V*t*; $n = rc$	$\Omega(G,x) = 2t \cdot x^{2cn/t}$	$t = div\ c$

In Table 3, the V-twisted isomers (T(4,4)S, case 2 and T(4,4)R, case 8) behave regularly, within the range of *n*=*rc*, according to the only relation, written in these entries. For no twisting, *t*=0 and H*t*=V*t*.

The H-twisted isomers are more complicated in the Omega description, and more cases are encountered.

The formulas are obeyed for t= *div c* or *div c,n*, or *div n* i.e., the divisors of the net parameters. Multiples of these divisors show the same expression for the polynomial and identical values of *CI* index. It is no mater if the objects generated by the TORUS software are distinct topological objects or not; the divisors of the net parameters will always provide distinct polynomials and also distinct *CI* index values. The first derivative provides the number of edges in the graph.

The dependence by t of the omega polynomial coefficients can be informative with respect to the helicity of tubular nanostructures.

Conclusions

Omega polynomial $\Omega(G,x)$ counts the qoc strips of all extent in G. The qos strips consist of the topologically parallel edges cut off by a cutting procedure. Close formulas for the calculation of the Omega polynomial in toroidal T(4,4)S/R objects, in H/V twisted embeddings, were derived.

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