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Omega and Theta Polynomials in Conical Nanostructures

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Abstract. Omega $\Omega(G,x)$ and Theta $\Theta(G,x)$ counting polynomials, defined on the ground of *quasi-orthogonal cut "qoc"* edge strips and edge equidistance, respectively, are calculated on conical objects. The building of nano-cones and derived hourglasses is discussed in connection with their polynomial description.

1. Introduction

Conical nano-structures are known in the literature as: nanocones, graphitic cones, molecular cones, or "buckycones". Surfaces of conical shape have been reported since 1968,[1] before the discovery of fullerenes. If a graphite sheet is divided into six sectors, each with an angle of 60º (Figure 1), and if m of these sectors (with m varying from 1 to 5) are deleted sequentially, with the dangling bonds being fused together, five classes of single-walled nanocones are obtained, with an angle α at the cone apex of 112.9º, 83.6º, 60.0º, 38.9º, and 19.2º. These values correspond to the formula:[2] $\alpha = 2\arcsin(m/6)$. One can add two extreme cases: (i) the graphene sheet, with all m = 6 sectors preserved (*i.e.*, a "cone" with an angle of 180º) and (ii) all m = 6 sectors are deleted, case in which a "cone angle" equal to zero is obtained (which corresponds to a nanotube capped at one end with a hemi-fullerene, as observed by transmission electron microscopy[3,4]).

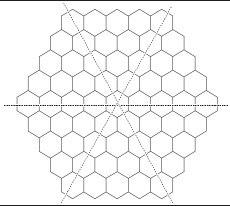


Figure 1. The six sectors on a honeycomb lattice.

In the hereafter text, only cones ending in the apex polygons of size s = 3 to 5, with no other polygonal defect of the graphite sheet, will be considered. The name of such objects includes: {[tip polygon]CONlength (of the cone body)}, in number of hexagon rows - Figure 2.

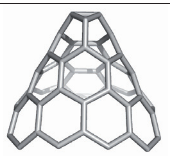
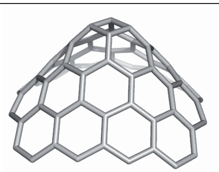
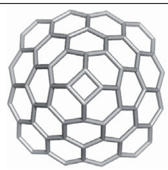
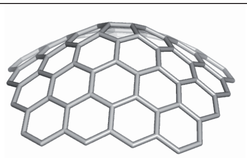
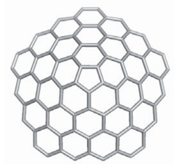
[3]CON3; v = 48	
	
[4]CON3; v = 64	
	
[5]CON3; v = 80	
	

Figure 2. Nanocones ending in a trigonal, tertagonal or pentagonal apex.

Conical zones may be involved in the construction of the DWT, suggested[5] to result by sealing, with an electron beam, a double-walled carbon nanotube DWNT in two distinct positions. Proposals of toroidal structures bearing polygonal defects are known since the pioneering times of nanoscience.[6-8] Such structures, of genus 1, including conical zones and called hereafter conetori, are built up by joining the cones with two tubes, one internal and the other external, of distinct diameters. Their name includes: {[apex:length]CT(junction, internal tube type, length), (junction, external tube type, length)}, the length being given in number of hexagon rows. The tube is either a H/Z (zig-zag) or V/A (armchair).[9]

The idea of the possible synthesis of this kind of tori originates in the experimental evidence of nano-peapods, a hybrid structure consisting of (coalesced) fullerene molecules encapsulated in single-walled nanotubes.[10]

Two conical units could be connected to form a fullerene, an hourglass (Figure 3), or a torus.

([5:2]CON(7H0); v = 160 ([5:2]CON(7H1); v = 170

Figure 3. Conical units joined to form hourglasses.

2. Counting Polynomias of Equidistant Edges

Let $G(V,E)$ be a connected graph with the vertex set $V = V(G)$ and edge set $E = E(G)$, without loops.

Two edges e = (1,2) and e' = (1',2') of G are called *codistant* (briefly: e *co* e') if for k = 0,1,2,… there exist the relations: d(1,1') = d(2,2') = k and d(1,2') = d(2,1') = k+1 or vice versa.[11] Note that the "*co*" relation is not always transitive (*i.e.*, if e *co* e' and e' *co* e'' *then* e *co* e''). Let $C(e) = \{ e' \in E(G);\ e' \ co\ e \}$ denote the subset of all edges of G which are codistant to the edge e. If all the elements of $C(e)$ are codistant to each other then $C(e)$ is called an *orthogonal cut "oc"* of G.

If any two consecutive edges of a cut edge sequence are codistant and belong to one and the same face of the covering, such a sequence is called a *quasi-orthogonal cut "qoc"* strip. This means that the transitivity relation is not necessarily obeyed. Any *oc* strip is a *qoc* one but the reverse is not always true.[12]

Recently, Diudea[12,13] has proposed the *Omega* $\Omega(G,x)$ polynomial for counting the *qoc* strips in *G*:

$$\Omega(G,x) = \sum_c m(G,c) \cdot x^c \tag{1}$$

with *m*(*G*,*c*) being the number of strips of length *c*. The summation runs up to the maximum length of the *qoc* strips in *G*.

On the same ground of *qoc* strips, another polynomial, called Theta ,$\Theta(G,x)$, was defined by Diudea:

$$\Theta(G,x) = \sum_c m(G,c) \cdot c \cdot x^c \tag{2}$$

Omega and Theta polynomials count *equidistant edges* in *G*; relation (2) is true only in graphs which are partial cubes,[xx] otherwise *m*(*G*,*c*), written as $m_\Theta(G,c_\Theta)$, counts the the number of sets of equidistant edges of cardinality c_Θ and the polynomial can be re-written as:

$$\Theta(G,x) = \sum_c m_\Theta(G,c_\Theta) \cdot x^{c_\Theta} \tag{3}$$

The Omega 1.1 software program[14] enabled us the calculation of the two discussed polynomials.

3. Counting Polynomials in Conical Nanostructures

The Omega and Theta polynomials are calculated on hourglasses, with the parameters presented in Figure 4. There are several cases for which we were able to derive close analytical formulas: (a) hourglasses without tube (with only heptagons needed to the two conical domains and no rows hexagons between); (b) hourglasses with tube and one row hexagons in the skirt and (c) hourglasses with modified tube and skirt (see below).

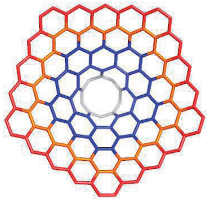


Figure 4. Conical units joined to form an hourglass (with the meaning of symbols: p=size apex polygon; n=no. hexagons rows in the skirt; t =no. hexagons rows in the tube; p=5; n=3; t=0).

3.1. Omega Polynomial

(a) Hourglasses without tube. In this case, formula depends only of the p and n parameters (Table 1). Below the formula, some examples are given.

Table 1. Hourglasses without tube

$$\Omega(p,n)=4px^1+6px^{n+1}+2p\sum_{i=1}^{n}x^{n+2+i}$$	
p=5	
$20x^1+30x^2+10x^4$	n=1
$20x^1+30x^4+10x^6+10x^7+10x^8$	n=3
p=4	
$16x^1+24x^2+8x^4$	n=1
$16x^1+24x^4+8x^6+8x^7+8x^8$	n=3
p=3	
$12x^1+18x^2+6x^4$	n=1
$12x^1+18x^4+6x^6+6x^7+6x^8$	n=3

(b) Hourglasses with tube and one row hexagons in the skirt. In view of preserving the symmetry of formulas, the parameter n was also included (Table 2).

Table 2. Hourglasses with tube and one row hexagons in the skirt

$$\Omega(p,n,t)=2px^1+6px^2+tx^p+2px^{t+1}+2px^{n+3}$$	
p=5	
$10x^1+30x^2+10x^3+10x^4+2x^5$	t=2; n=1
$10x^1+30x^2+20x^4+3x^5$	t=3; n=1
p=4	
$8x^1+24x^2+19x^4$	t=3; n=1
$8x^1+24x^2+15x^4+8x^8$	t=7; n=1
p=3	
$6x^1+18x^2+8x^3+6x^4$	t=2; n=1
$6x^1+18x^2+5x^3+6x^4+6x^6$	t=5; n=1

(c) Hourglasses with modified tube and skirt. In this case, all the three parameters are present (Table 3).

Table 3. Hourglasses with modified tube and skirt

$$\Omega(p,n,t) = 2px^1 + 6px^{n+1} + tx^p + 2px^{t+1} + 2p\sum_{i=1}^{n} x^{n+2+i}$$

p=3	
$6x^1+18x^2+8x^3+6x^4$	t=2; n=1
$6x^1+8x^3+18x^4+6x^6+6x^7+6x^8$	t=2; n=3
p=4	
$8x^1+24x^3+11x^4+8x^5+8x^6$	t=3; n=2
p=5	
$10x^1+30x^3+10x^4+13x^5+10x^6$	t=3; n=2

3.2. Theta Polynomial

In case of Theta polynomial, the formulas were derived for each case of apex polygon type. The domains of working are indicated in tables.

(a) Hourglasses without tubes (Table 4)

Table 4. Hourglasses without tube

$$\Theta(p,n) = 2px + 2px^2 + 20nx^{n+1} + 2p\sum_{i=1}^{n-1}(n+2+i)x^{\sum_{i=1}^{n-1}(n+2+i)} + 6p(n+1)x^{2(n+1)}$$

p=5	
$10x^1+30x^2+20x^3+60x^4$	n=1
$10x^1+10x^2+60x^4+20x^5+60x^6+70x^7+120x^8$	n=3
p=4	
$\Theta(p,n) = 2px + 2px^2 + 2p\sum_{i=1}^{n-1}(n+2+i)x^{\sum_{i=1}^{n-1}(n+2+i)} + 10p(n+1)x^{2(n+1)}$	
$8x^1+8x^2+80x^4$	n=1
$8x^1+8x^2+48x^6+56x^7+160x^8$	n=3
p=3	
$\Theta(p,n) = 2px + px^2 + 6px^{n+1} + 2px^{\sum_{i=1}^{n}(n+2+i)}$	
$6x^1+21x^2+6x^4$	n=1
$6x^1+3x^2+18x^4+6x^6+6x^7+6x^8$	n=3

(b) Hourglasses with tube and one row hexagons in the skirt (Table 5).

Table 5. Hourglasses with tube and one row hexagons in the skirt

p=4	
$\Theta(p,t) = 2px + (20p + 4(t-4)x^4 + 4px^8 + 4px^{10} + 8px^{12} + 2p(t-5)x^{14};\ t \geq 5$	
$8x^{+}84x^4+16x^8+16x^{10}+32x^{12}$	*t*=5
$8x^1+104x^4+16x^8+16x^{10}+32x^{12}+40x^{14}$	*t*=10
p=3	
$\Theta(p,t) = 8px^2 + (6+3t)x^3 + 8px^4 + 4px^6 + 4px^8 + 4px^9 + 2p(t-3)x^{10};\ t \geq 3$	
$24x^2+15x^3+24x^4+12x^6+12x^8+12x^9$	*t*=3
$24x^2+24x^3+24x^4+12x^6+12x^8+12x^9+18x^{10}$	*t*=6

Conclusions

Omega $\Omega(G,x)$ and Theta $\Theta(G,x)$ polynomials count equidistant edges in a graph; their definitions are based on the *quasi-orthogonal cut* qoc strips of all extent in *G*. Close formulas for the calculation of the two polynomials in conical nano-objects were derived.

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