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Hyper-Tubes of Hyper-Cubes

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ABSTRACT Hyper-tubes consisting of hyper-cubes of *n*-dimensions were designed and formulas for substructures of vary dimensions established.

KEYWORDS graph • n-cube • hyper-tube • hyper-torus • n-dimensional space

1. INTRODUCTION

The macroscopic universe, as well as the microscopic realm of molecules and crystals had required, in the last years, knowledge about spaces of dimensions higher than three. The aim of finding *n*-space domains surrounded by the usual Euclidean 3D-space, in complex chemicals (mineral or synthetic ones) promoted important works towards a systematic design of new *n*-dimensional hyper-structures. Let, first recall some basic mathematical notions.

A ***convex hull*** (or envelope) [1–3] of a set X of points in the Euclidean space is the smallest convex set that contains X. A set of points is called convex if it contains all the line segments connecting each pair of these points. The convex hull of a finite point set $S \in \mathbf{R}^n$ forms a convex polygon, for $n = 2$, or, in general, a convex polytope in $\mathbf{R}^n$. Every convex polytope in $\mathbf{R}^n$ is the convex hull of its vertices.

Schläfli [4] 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 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. In the following, some details are given.

The ***n-simplex*** [1], with Schläfli symbol $\{3^{n-1}\}$, and the number of its k-faces $\binom{n+1}{k+1}$, is a generalization of the triangle or tetrahedron to any dimensions. A simplex is an n-dimensional polytope, which is the convex hull of its n + 1 vertices. 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*** [1] is a generalization of the 3-cube to n-dimensions and is also called an n-cube C(n). It is a regular polytope with mutually perpendicular sides, thus being an orthotope. Its Schläfli symbol is $\{4,3^{n-2}\}$ and k-faces are counted by $2^{n-k}\binom{n}{k}$.

The ***n-orthoplex* or cross-polytope**[1] has the Schläfli symbol $\{3^{n-2},4\}$ and k-faces $2^{k+1}\binom{n}{k+1}$; it exists in any n-dimensions as the dual of n-cube.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 polytopes, a formula, also due to Schläfli [4], is used

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

For n = 4, eq (1) reduces to the well-known Euler [5] 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.

2. RESULTS AND DISCUSSION

In two previous papers [6,7], the hyper-cube embedding in the torus surface, particularly the tori T(4,r) and T(4,r,s), according to Diudea's discretization procedure [8], was reported. In this paper, the formulas for the corresponding tubes (i.e. the open tori) are derived.

The number of k-cubes C(n,k) contained in the hypercube, C(n), can be calculated from the coefficients of $(2k+1)^n$ [1]

$$C(n,k) = 2^{n-k}\binom{n}{k}; \qquad k = 0,..,n-1 \tag{3}$$

The hyper-cube can be embedded in a cylinder (or a tube, see Figure), to provide, for example, a tube of section 4 (i.e. a cuboid) along its generator *r*; such a tube is denoted hereafter TU((4,*r*),C(*n*),TU(n+1)).

Theorem 1. The *k*-dimensional substructures of a hyper-tube TU((4,*r*),C(*n*),TU(n+1)) are counted from the hypercube C(*n* , *k*) substructures by formulas:

$$f_r = (r/2-1)/n \qquad \begin{matrix} f_k = (r/2) + k \cdot f_r \\ k = 0,1,..,n-1 \end{matrix}$$
$$TU((4,r),C(n),TU(n+1),k) = C(n,k)\cdot f_k \tag{4}$$
$$T((4,r),C(n),T(n+1),(k+1)) = r$$

Demonstration comes out from the data listed in Table 1. One can see alternation of figure count Sum(f_i) according to the Schläfli formula (1): zero for even TU-dimension and 2 for the even dimension Dim of the hyper-tube. It means that the elementary hyper-tube TU((4,*r*),C(n),TU(*n*+1)) is like the sphere (i.e. had the genus g = 0).

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

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

In a more complex hyper-tube (Figure, the right column); each unit in the tube TU((4,*r*,*s*),C(*n*),TU(*n*+1)) is an elementary hyper-torus T((4,*r*),C(*n*)T(*n*+1)) while there are s-units along the tube.

The following theorem will allow to understand the hyper-tube TU((4,*r*,*s*),C(*n*),T(*n*+1)) composition:

Theorem 2. The *k*-dimensional substructures of a hyper-tube TU(4,*r*,*s*),C(*n*),TU(n+1)) are counted from the previous dimensional substructures of the elementary hyper-torus T((4,*r*),C(*n*),T(*n*+1)) hyper-torus, by formulas:

$$TU((4,r,1),\mathrm{C}(n),TU(n{+}1),k)) = T((4,r),\mathrm{C}(n\text{-}1),T(n),k) + T((4,r),\mathrm{C}(n\text{-}1),T(n),(k-1)) \qquad (5)$$

$$TU((4,r,s),C(n),TU(n{+}1),k) = s \times TU((4,r,1),C(n),TU(n{+}1),k)) + T((4,r),\mathrm{C}(n\text{-}1),T(n),k) \qquad (6)$$
$$k = 0,1,..,n-1; n > 3$$

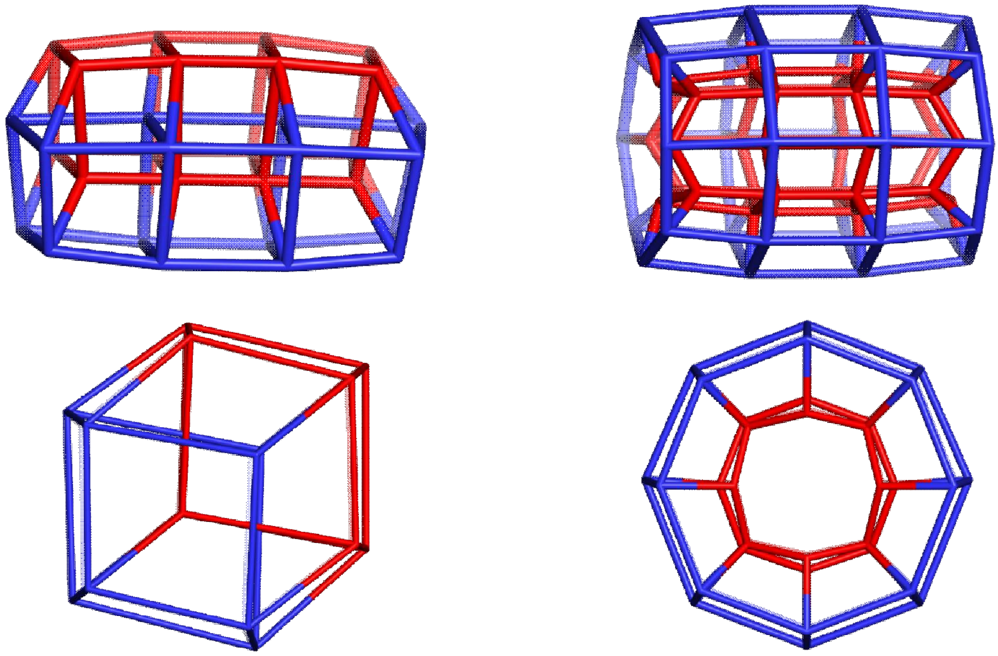

Figure 1. A hyper-tube TU(4,4),C(4),TU(5)).32 (left column) and a hyper-tubeTU((4,8,4),C(3),TU(4)).64 (right column)

Demonstration comes out from data listed in Table 2. Formulas work for any integer n>3. The all (+) sum of the substructures of the hyper-torus units can be evaluated by the formulas found at the bottom of this table.

Table 2. Figure count in the hyper-tubeTU((4,9,7),C(5),TU(6)).504.

Structure \ k	0	1	2	3	4	5	Sum(f_i)	Dim
TU((4,9,7),C(5),TU(6)).504	504	1692	2214	1413	441	54	0	6
T((4,9),C(4),T(5)).72	72	180	162	63	9	-	0*	5
	-	72	180	162	63	9	-	-
TU((4,9,1),C(5),TU(6)).72	72	252	342	225	72	9	0**	6
TU((4,9,1),C(5),TU(6))x6	432	1512	2052	1350	432	54	-	-
+ T((4,9),C(4),T(5)).72	72	180	162	63	9	0	-	-
Sum	504	1692	2214	1413	441	54	0	6

*All+Sum(f_i)=r×2×3^(n-2)=486, for r=9; n=5
**All+Sum(f_i(T(4,r,1))=r×4×3^(n-2)=972, for r=9; n=5; n=dimension of the hyper-cube.

Note the difference between the hyper-cube and TU((4,*r*),C(n),TU(*n*+1)) on one hand and the hyper-tube TU((4,*r*,*s*),C(*n*),TU(n+1)) on the other hand: the figure sum, Sum(f_i), in the two objects follows the formula (1) (with alternating 0 and 2 for even and odd *n*-dimension, respectively) while the last structure provides zero (see Table 2), irrespective of *n* parity. This is also true for the hyper-tori embedding hyper-cubes, because both cylinder and torus have the genus $g = 1$ [9].

3. Computational Details

The design and properties of the studied structures was performed by our original Nano Studio [10] software program.

4. Conclusions

Multi-shell clusters appearing frequently in minerals or synthetic chemicals [11] (e.g. some clusters of 13-atoms, like: MaMb12 or M13, M=Fe, Pd, Ru, Rh, showing giant magnetic moments [12,13], or simple molecules as B4Cl4, $Co(CO)_4^-$.etc. can be considered to belong to space dimensions higher than three. Knowledge on such higher dimensional clusters could be of interest in structure elucidation efforts.

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