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Steiner systems (t-(v, k, λ) schemes) and special features of the nanostructures symmetry description

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Abstract

The situation with description of nanostructures is much more complicated than, for example, for crystalline materials. In this case we have not used the classical crystallography. The order specified in a finite ordered set can always be enhanced to a linear order, which enables us to construct the incidence matrix for this set and, hence, to change over to algebraic constructions (including the aforementioned constructions of the projective geometry).

Keywords: Algebraic constructions; Nanocomposites; Chemical properties; Traditional ceramics; Functional applications

1. Introduction

Nanostructures essentially to not be reduced to a crystal (association of crystals) nanoscales, as. As against a crystal representing a transmitting lattice of associations coordination polyhedron, in nanostructure requirements Euclid's, compactness, to connectivity and cogerents it is transferred on a local level and are realized at assembly (the certain fundamental varieties) geometrical structural complexes of the device and law of the fibration space. An adequate mapping of symmetry of structures in the condensed state, ranging from nanostructures to quasicrystals and crystals, requires that generating varieties and the law of their union be described in the context of a local approach. In this approach a structure is assembled from a set of peculiar generating clusters, and the assembly laws are defined by the geometric structural complex themselves and topological properties of space.[1–10] Each geometric structural complex may be matched with a point or vector variety (finite or infinitely geometric-an atom-generated sublattice).[6] The latter implies that in the construction of local groups and local isomorphism, consideration must be given to their associated algebraic varieties and, eventually, to representations of a given geometric lattice by closed subsets of the algebraic system (coordinatisation).[7–9]

Sphere packings and algebraic lattices are closely linked to the problem of decoding and finding optimal codes. Therefore, well-studied lattice codes may be used in the construction of non-crystalline systems. Linear codes are normally used, and, in particular, binary codes—a set of binary vectors (code words) of length n (having n coordinates), consequently a set from F_2^n, where F_2 is a finite Galois field with two elements. Similarly, q-nary code is a subset in F_q^n, where F_q—is a finite filed with q elements (q—a power of a prime number). Transition from geometric constructions to algebraic ones is determined by the fact that non-trivial solutions of homogeneous equations defined over a Galois field exactly corresponds to a set of hyperplanes in the Galois space corresponding to the given equations. The Galois field $\mathrm{GF}(q) = K$, where $q = p^r$ (p is a prime number), can be viewed as a vector space over the subfield $P = \mathrm{GF}(p)$.

2. Construction of the finite projective plane and t-scheme

If there are manifold from v-elements (points), a t-(v, k, λ)-scheme is a varies k-submanifolds (blocks) so that each t-submanifolds be contained in the λ blocks. Of special value are projective t-schemes ($t = 2$, 3), for, as is known,[4] for $n \geq 3$ every axiomatically defined geometry is isomorphic to a projective geometry over some field. A more general case is given by t-(v, k, λ)-schemes.[6] If $\lambda = 1$ then the scheme is called a Steiner system $S(t, k, v)$. In the case of point varieties and corresponding points ($t = 1$) we have $bk = vr$, so that every point belongs to r

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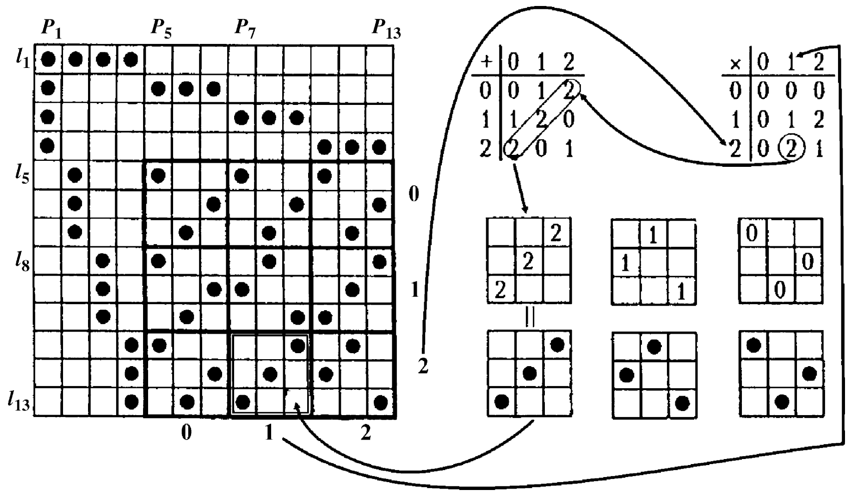

Fig. 1. Construction of the finite projective plane PG(2, 3) incidence table of the Galois field GF(3).[12–14] Indices 2 and 1 of the square C^{21} (double lines) coincide with elements 2 and 1 of the multiplication table (x) row and column of the Galois field GF(3) = {0, 1, 2}. The product of these elements is defined by element 2, whose distribution in the addition table (+) GF(3) does represent the distribution of incidence signs over the square C^{21}. The squares C^{mx}, c, m or x equal to 0 are the same and represent the distribution of 0 over the addition table GF(3). A square from from 3^2 squares C^{mx}, $m, x = 0, 1, 2$ represents the Q-interiors of the table.

blocks. Usually the blocks are taken to be code words of given weight, and every block $B \subseteq M$ can be represented by its characteristic vector $(c_1 \ldots c_v)$, such that $c_i = 1$ if $i \in B$ and $c_i = 0$ if $i \notin B$. Thus, t-scheme is a binary code of length v, whose every word has weight k. Such an approach allows one to link said characteristic vectors to characteristic classes depending on the manifolds used and on the given type of discrete fibration in constructing non-crystalline structures within the local approach. A special interest in t-schemes (t = 2, 3) is caused by their relation to finite projective geometries (Fig. 1, Table 1) and the presentation of groups by geometric graphs (sets of points and intervals connecting them according to certain rules). Every finite graph can be included in some surfaces like vertices and edges of a map decomposing a closed surface; therefore, there is a correspondence between authomorphism groups of the graph and the map. For two-surfaces we can obtain in this way all known polyhedral decompositions in E^3.

An ovaloid is a $(q^2 + 1)$-point subset of the projective space of order q in which no three points are collinear. Such planes are isomorphic to a sphere given in the Galois space of order q as point sets defined by equations of second degree. From the features of construction of Galois planes it follows that for planes of odd order the number of tangent planes to the ovaloid with a common point is $q^2 + q$, and the number of planes containing more than one point is $q^3 + q$, so that the total number of such planes is $(q^2 + 1)(q + 1)$. Thus, the use of the ovaloid over the coordinate field GF(2) allows one to obtain points of the finite affine plane of the corresponding order, which, in its turn, can be put into correspondence with the root system of the respective semisimple algebra. Apart from finite projective planes that use the condition ($t = 2$, $\lambda = 1$, $v = q^2 + q + 1$, $k = q + 1$), for t-(v, k, λ) scheme one can use a projective construction of the Mobius plane (M) and ovaloid types.[11] For an ovaloid with $t = 3$, we have $v = q^2 + 1$, $k = q + 1$ ($\lambda = 1$). The values M_i themselves, related to M-plane (t = 3) allow one to consider possible projective configurations[11] as well as. t-Schemes allow us to define a major part of deterministic constructions, including maximal ones, related to the groups of substitutions; in particular, to groups of collineations, to which, as is known, the finite projective geometries are reduced.[5] In the general form each t-scheme is at the same time a t'-scheme for any integer $t (2 \leq t' \leq t)$, so that at $t' = t - 1$, $\lambda' = \lambda((v + 1 - t)/(k + 1 - t))$, which does make it possible not to restrict one's consideration to PG(2, q) in constructing algebraic constructions rather than employing t-(v, k, λ)-scheme to deduce, say, rod substructures.

The cluster shown in Fig. 2b and c has D_3 symmetry and is included into FCC lattice. Thus, if the considered table incidence PG(2, q) = $S(2, q + 1, q^2 + q + 1)$, q = 2, 3, 4 defined the graphs of special clusters, namely, those of diamond-like structures, the sub-table incidence $S(3, q + 1, q^2 + 1)$, q = 3 defines the graph of

Table 1
System Steiner finite geometries

q	$t = 2$, $v = q^2 + q + 1 = b$, $r = q + 1 = k$				$t = 3$, $v = q^2 + 1$, $k = q + 1$			
	PG(2, q)	$q^2 + q + 1$	$q^3 + q^2 + q + 1$	$S(2, k, v)$	$q^2 + 1$	$b = q^3 + q$	r = $q^2 + q$	$S(3, k, v)$
2	PG(2, 2)	7 ($q^2 + q + 2$) = 8	18 = 3 × 6	S(2, 3, 7) b = 7, r = 3	5 ($q^2 + 2 = 6$)			
3	PG(2, 3)	13	40 = 4 × 10	S(2, 4, 13) b = 13, r = 4	10	30	12	S(3, 4, 10) b = 30, r = 12
4	PG(2, 4)	21	90 = 5 × 18	S(2, 5, 21) b = 21, r = 5	17 ($q^2 + 2 = 18$)	68	20	S(3, 5, 17) b = 68, r = 20
5	PG(2, 5)	31	186 = 8 × 31	S(2, 6, 31) b = 31, r = 6	26	130	30	S(3, 6, 26) b = 130, r = 30
7	PG(2, 7)	57	400 = 8 × 50	S(2, 8, 7) b = 7, r = 3	50	350	56	S(3, 8, 50)
11	PG(2, 11)	133	12 × 122	S(2, 12, 133) b = 133, r = 12	122	1342	132	S(3, 12, 122) b = 1342, r = 132

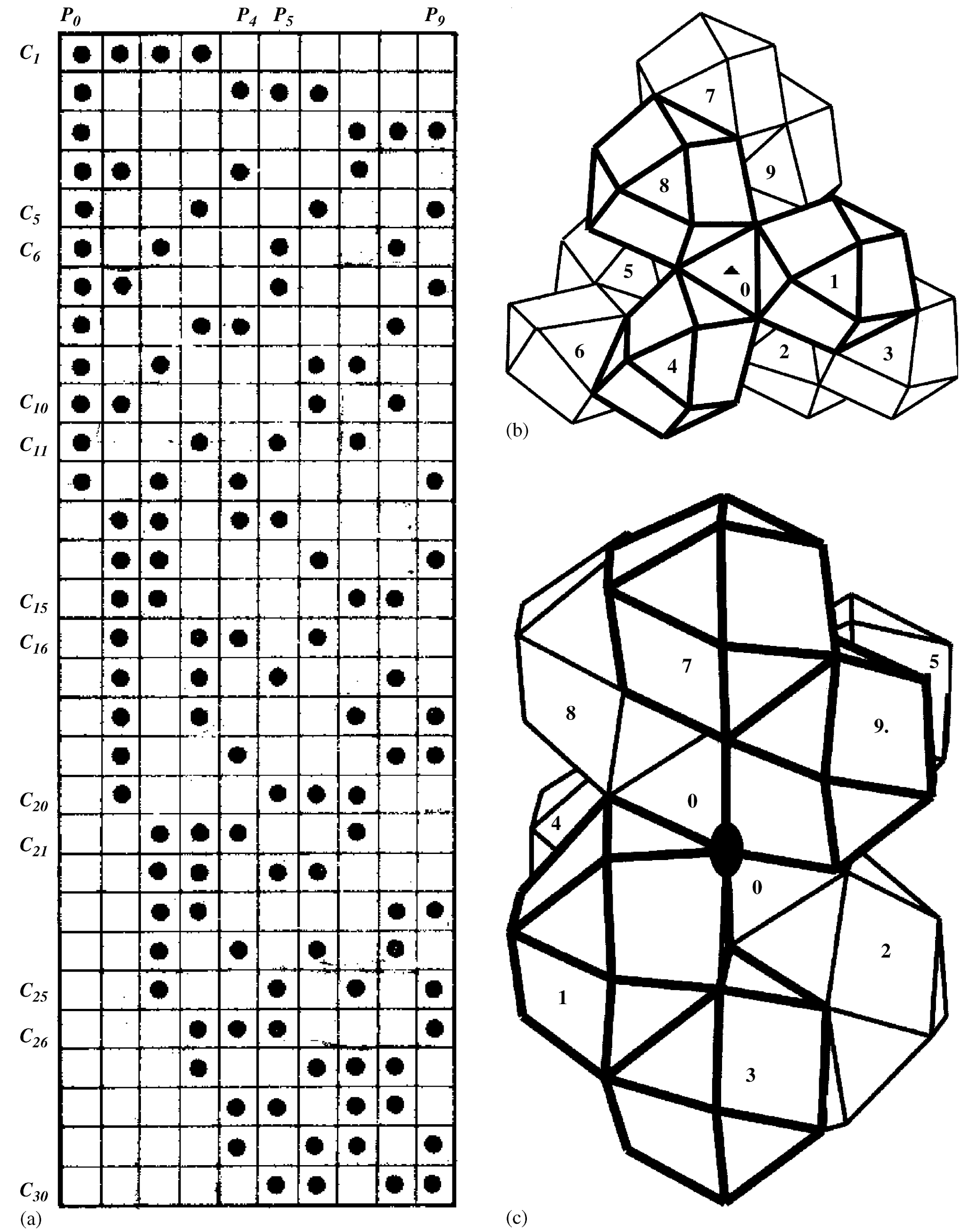

Fig. 2. Table incidence of plane Mobius order 3,which determined nine cubooctahedral assembled from central. cubooctahedron. (a) Table incidence of plane Mobius (inverse plane) order 3 as 3-(10, 4, 1)-scheme. (b) and (c) Nine cubooctahedral assembled from central. cubooctahedron from FCC. Three-fold (b) and two-fold (c) axes of all cluster coincides with the axes of central. cubooctahedron.

a special cluster of a metallic structure. A more detailed a priori derivation of special clusters using t-(v, k, λ) schemes will be considered separately.

3. *t*-Scheme and fibre space

In contrast to group representations, which give in general a realization of arbitrary transformations, algebras correspond to linear transformations. If G is a freely acting group in a fiber space, it is a fiber substitution group and coincides with a monodromy group acting in the fiber (covering). Constructing certain nanostructures as algebraic constructions requires one to make use of certain types of the Hopf fibration $S^7 \rightarrow S^4$ (fibre S^3) and the root lattice E_8[8–10] (Fig. 3). For the Hopf fibrations it is important that using polytopes as fiber spaces guarantees the conservation of the local minimum property of manifolds in the fiber.

A S^7 sphere can be viewed as a fibre space to be defined by an algebraic construction of smooth fibration involving a fibre space (variety), a fibre base (variety) M, a projection (smooth mapping of a fibre space into the base), a fibre (variety) F, a structural group G representing a group of fibre transformations, a fibre structure (i.e. the law under which the base is covered by domains U_α over which coordinates of the direct product $F \times U_\alpha$

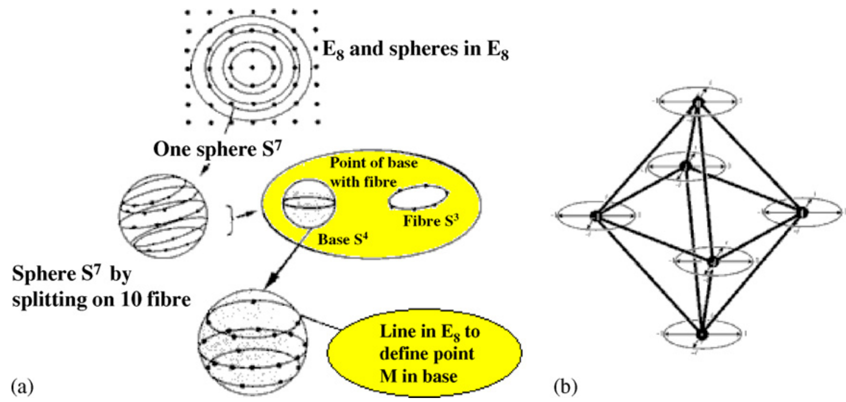

Fig. 3. Hopf fibration: (a) model for the Hopf fibration $S^7 \to S^4$ (fibre S^3) for the first coordination shell in E_8.[10] (b) Model for the Hopf fibration $S^3 \to S^2$ (fibre S^1) for the polytope {3, 4, 3}. Six base points form an octahedron. Four points of each fibre make up a square.

are embedded in complete preimages using diffeomorphisms). Fibration sections are the function $\Psi(x)$ taking on values at the point $x \in M$ in the fibre F_x determined over x^2. If the realisation of group G is given as a group of smooth transformations of a F' fibre other than F, then from any fibration with group G and fibre F one can build a fibration referred to as associated. Indeed, the fibre structure is defined by agglutination functions or mappings of $T^{\alpha\beta}$: $U_{\alpha\beta} \to G(U_{\alpha\beta} = U_\alpha \cap U_\beta)$, which could always be realised as right shifts in the group G itself. The latter is due to the fact that a particular fibre type is of no importance. One can always build a fibration associated to a source one by using, say, a variety of fibre sections. Thus, the problem of fibration classifications is to classify the principal fibrations (obtained from the free operation of group G in the space of fibrations), since any fibration may be defined as that associated with some principal one.[10] Additional possibilities are provided by rod substructures, whose characteristics are defined with b and r for the corresponding t-schemes in construction of discrete fibrations. A general approach using t-schemes in construction of trivial fibrations employs multiplication of two integers related to root systems of semisimple algebras or their subsystems, corresponding to various.

4. Algebraic construction and rod-substructure

Polytope substructures which can be embedded in E^3 with minimal distortions represent rod substructures. The maximum polytope part that can be embedded in E^3 with minimal distortions represents a rod substructure. Among the axes of the said rod substructures are non-integer axes (rod substructures), along with integer ones (crystallographic and non-crystallographic). In this case helicoids and a dense packing of spherical objects correlate with each other.

Using the multiplication laws for those algebras, one may use discrete fibrations line $S^3 \to S^2 \times S^1$. For example, given the direct product $S^i \times S^j$, it contains a bouquet of the type $S^i \cup S^j$, and so on. Associated fibrations may be of two types: trivial (when one of the coefficients used is scaled by an integer) and

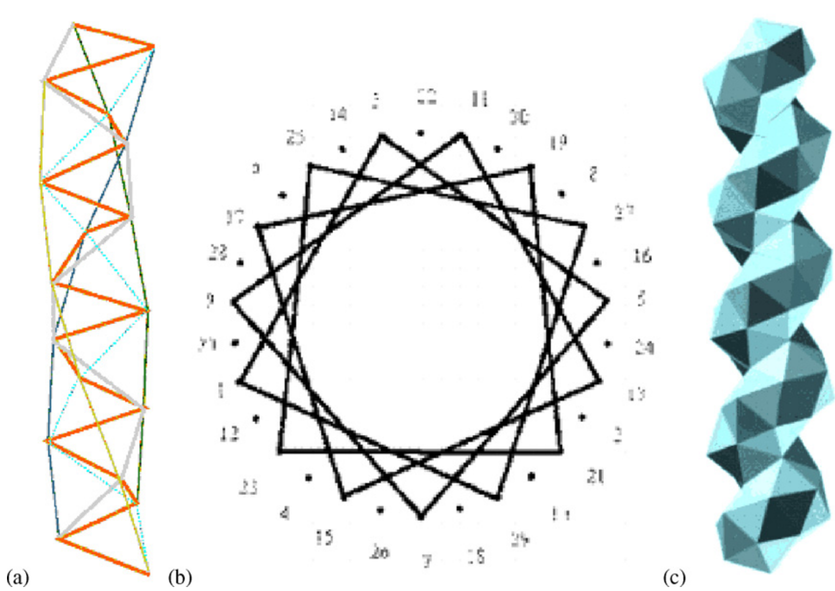

Fig. 4. Spiral 15/4: (a) two spirals 15/4 (dotted and grey line) in the Bernal chain made up of tetrahedra. Each edge of spiral 15/4 is shared by two tetrahedra, spiral 30/11 is indicated by a thick line. (b) Stellated polygon 15/4 whose vertices "cover" half of polygon 30/11 vertices. (c) Rod structures assembled from icosahedracentres form spiral 15/4.

those where k/r is not integer. In this case one may use a bouquet-like construction $S^1 \cup S^2$ or $S^2 \cup S^2$ ... and single out certain points (elements). In a simplified form, whenever it is necessary to construct a set.

As was shown before,[17] the Bernal chain has edges of three types, namely those belonging to one, two, and three tetrahedra. The first-type edges form three spirals 10/1 (Fig. 4c), the second-type edges make up two spirals 15/4 (Fig. 4) and the third-type edges, spiral 30/11. All the mentioned spirals correlate with plane involutes of a cylinder and a torus from the Hopf fibration for the polytope $\{3, 3, 5\}$. In, Ref.[15] [15] the authors show a possibility to describe spiral biological structures and quasicrystals in the topological language of the Hopf fibration. It can be shown that for the complete symmetry description of the non-crystallographic densest packing, it is necessary to use associated fibrations for the polytope $\{4_{21}\}$, since its 240 vertices represent the first coordination shell of lattice E_8. The fundamental theorem, which is likely to define distinctive feature of "axial" substructures, will be a theorem regarding the existence of a tubular neighborhood.[2]

It is also shown that axis 15/4 becomes realized as a spiral chain of regular icosahedra (Fig. 4c). It is impossible to explain phase transitions in nanostructured systems without looking at non-integer axes, while their "appearance", as such, in experimental data (primarily, following the results of high-resolution electron microscopy) is kind of indicative of the necessity of using a fibre space instrument and the impossibility to restrict ourselves to crystallographic groups in order to describe finite lattices (nanocomposites). The associated fibrations, in particular the Hopf fibrations for $\{4_{21}\}$ ultimately define not only axes described in Ref.[15] [15] but other non-integer axes as well, such as 10/3, 20/7, 12/5, 18/5, 14/3, 15/4, 8/3, 28/13, 24/5.[8] It is obvious that under this consideration, non-integer axes give an idea of the "packing" of given polyhedra in certain algebraic constructions denoted as rod substructures. Thus, a transition from translation assembly of structures to their assembly under the laws of fibre spaces (and, hence, a transition from crystallographic lattices to finite ordered ones) lifts crystallographic bans on the appearance of axes of the order $n \neq 2, 3, 4, 6$, in particular those of order 5, 10, and non-integer ones.

Upon one-sheeted cover for a fibre group each element (point of the base) should be laden with a minimum k points of the fibre, which define k–c vectors. A set of bk points possessed by b fibres can in the general case be split into bk (overlapping) sets having k–c vectors each. Such sets can be viewed as intransitive domains for a cyclic axis of the order: let b and N be the numbers of the base points (characteristic of the vector field given on the base) and of the fibre, respectively, then $b \times N = L(N)$ is the number of the substructure $\{4_{21}\}$ elements, the number coinciding, on occasion, with the number of vertices of the corresponding n-dimensional polyhedron.

Consider some examples of the associated discrete Hopf fibrations defined by various (geometrically conditioned) splitting of the fibre N in the fibration with $L(N) = 120$. The fibre structure is defined by a gauge non-Abelian 24-element group H (Gurvitz's group) containing no subgroup of order 12. The latter implies that the fibre $\{3, 4, 3\}$, which gives the following splitting of its vertices. Having generalised, we obtain that depending on the number of points for the base $e = L(N)/N$, splitting of the fibre N and cover for the fibre group, the fibration for the substructures $\{4_{21}\}$ defines an axis of the order: The choice of $L(N)$, N, m and c practically defines one of the subsystems of the E_8 root vectors, which complies with one or other algebra or its root lattice:[18]

$$\frac{p}{q} = \frac{L(N)/\gamma}{N - mc} \tag{1}$$

where γ, $c = 1, 2$; m is the non-trivial divisor mismatching N. It is the next example:

$$24 = 16 + 8 = 4.4 + 4.2 = 4(4 + 2), \quad \text{for which} \quad m = 4,$$

$$c = 2 \quad \textit{and} \quad \frac{p}{q} = \frac{120/2}{24 - 4(2)} = \frac{60}{16} = \frac{15}{4}. \tag{2}$$

The "edge figure" of the $\{3, 4, 3\}$ is the joining of three octahedra along the common edge. This cluster has 11 vertices, therefore this gives the following breakdown (Fig. 4b):

$$24 = 2(11 + 1), \quad \text{for which} \quad m = 2, \quad c = 1 \quad \text{and}$$

$$\frac{p}{q} = \frac{120/2}{24 - 2} = \frac{60}{22} = \frac{30}{11}. \tag{3}$$

In the case under consideration polytopes or other point or vector varieties are used to construct a fibre space over whose base one can preset sufficiently intricate functions (fields, algebras) topologically related to distinctive features of a fibre in the Hopf fibration for the substructures $\{4_{21}\}$. The non-integer axes (1) give, in the context under discussion, an idea of the "packing" of the substructures $\{4_{21}\}$ in certain algebraic constructions, in particular in rod substructures.

5. Structural realization of *t*-scheme

For the given algebra and the root lattice E_8 the ring of invariants have a basis of homogeneous polytopes of degrees 2, 8, 12, 14, 18, 20, 24, 30, and the orbit of its isomorphism group is its spherical seven-scheme. Therefore, it is appropriate to consider v-schemes for $v = 4, 6, 8, 12, 14$ and the values of μ for known polytopes, which, in their turn, correspond to coordination spheres of the E_8 lattice and its sublattices. It is important to note that for $\mu k/r$-the number of points per conditional unit cell b is, in certain sense the number of such unit cells characterizing the given finite system—a nanostructure. Upon exclusion, as it has been considered previously,[5,8] one may use a general formula like $L = \mu[\alpha(v - \beta) + \alpha\beta]$, which leads to expressions like $\mu v/\alpha(v - \beta)$ or $\mu v/2\alpha(v - \beta)$. Since k/r is not an integer, while bk/r, b, μ, v are integers, in constructing associated fibrations $L = \mu v$ one may use b as the base, for mapping of base a local section U_i ($i = 1, \ldots, b$), and a fibre $-\mu k/r$. The simplest way to retain validity of the formulas above is to use $r = v - \beta(\mu\alpha v = L)$, therefore fixed $\alpha\beta$ points and a summing up in fibre (at a fibre-block are the μk elements for expressions $\mu k/r$ and $b\mu k/r = \mu v$. The latter de facto gives the construction law as a non-integral axis or a rod substructure.

As an example consider a case of 24 polytope $-L=24$, $\mu=4$ ($6\times4=24$) for the decomposition $2\times5+2=2(5+1)$, which corresponds to $\alpha=2$, $\beta=1$ and $r=5$. The necessary t-scheme is 2-{6,3,2}, which generates a non-integral axis 12/5 for $b=10$ ($4\times6/2\times5=12/5$). The next example, related to the polytopes {120} and {240} and decomposition $2\times11+2=24$, is related to the type 2 t-scheme-{12,3,2}, for which with $v=12$, $\mu=10$, $r=11$ and $b=44$, can obtain a rod substructure characterized by a non-integral axis 30/11 ((10×3)/11 = 30/11 or (10×12)/44 = 30/11).

Let us give also several examples of t-schemes for $k/r=1$ and $k/r=1/2$:

- 2-{4,3,2}, for $\mu=6(6\times4=24)$ and $v=4$, $b=4$, $r=3$ can obtain six-axis.
- 2-{6,5,4}, at $\mu=4(6\times4=24)$ and $v=6$, $b=6$, $r=5$ can obtain four-axis.
- 2-{5,4,3}, for $\mu=4$ ($5\times4=20$) and $v=5$, $b=10$, $r=8$ obtain 4(2)-axis or for $\mu=6(5\times6=30)$ can obtain 6(3)-axis.

For S(3, 4, 10) characterized by $v=10$, $b=30$, $r=12$, for 112-polytope ($\mu=60$) for six-leaf covering one may obtain a root substructure characterized by a (60×4)/(6×12) = 10/3 axis. S(2,3,7)—a Steiner system for $t=1$, characterized by $v=7$, $b=14$, $r=6$ or 2-{7,4,2}, characterized by $v=7$, $b=7$, $r=4$, respectively, for 14 and 28-sets ($\mu=2$) one can obtain a two-axis, and for 112 or 224-sets a eight-axis, for example.

Of interest also are polytope-related variants, when the following t-schemes are used. 3-{10,6,5}, characterized by $v=10$, $b=30$, $r=18$, for 600-polytope ($\mu=60$) for six-leaf covering one can obtain a (6×60)/(6×18) = 10/3 axis, and for 480-set ($\mu=48$)—8/3-axis, respectively. For the set of elements related to polytopes {120} and {240}, B for S(2, 3, 10) with $b=30$, $r=9$ to obtain for $\mu=24$ ($24\times10=240$) and $\mu=12$ ($12\times10=120$) eight- and four-axes, respectively. For the type 2 t-scheme {14, 7, 6}, for which $b=26$, $r=13$, to obtain for $\mu=4$ ($8\times14=112$) a rod substructure, characterized by a 28/13 axis.

In using complexification it should be taken into account that the complex space C^n admits locally[16] and m-leaf cover. For simple singularities of the groups A_k, D_k, E_6, E_7, E_8, the bifurcation diagrams of zeros are diffeomorphic to the manifolds of non-regular orbits (MNO) of reflection groups of the same name, with two smooth strata for each of A_4, D_6, E_8, the traces of bifurcation diagrams of zeros on which are diffeomorphic to MNO of non-crystallographic groups H_2, H_3, H_4 respectively. It has been shown,[16] that the set of orbits for such diffeomorphisms are cylindrical along the higher weight coordinates (which correlates with the used algebraic constructions in the form of rod substructures). One may limit consideration for the cover C_{n+1} (two-leaf), so that covering space (having symmetry A_1) may be cylindrically extended in C^{n+1}, obtaining (as pointed out above) at zero a frontal singularity of the D_{n+1} type (consequently D_4 for C_4).

For more complicated cases, for example, six-leaf cover, one may use the following t-schemes. S(3,4,8), characterized by $v=8$, $b=14$, $r=7$, for 240-set ($\mu/6=5$) one may obtain a 20/7 axis upon decomposition $(3\times7)+3=24$ (one may use 2-{8, 4, 3} characterized by $v=8$, $b=28$, $r=14$). Similarly, other t-schemes may be used to obtain 15/4 and 40/9 axes in large polytopes. For this purpose one may use S(5,8,10) for which $b=90$, $r=72$ to obtain for six-leaf cover $\mu=240$ ($240\times10=2400$—a polytope related to the second coordination sphere E_8) a 40/9 axis. Similarly, for 2-{5, 3, 3}, characterized by $v=5$, $b=20$, $r=12$ in 24-leaf cover and $\mu=72$ ($5\times72=360$—polytope) one obtains a rod substructure characterized by a 15/4 axis.

There is one more variant of the usage of t-schemes, related to fullerene-like structures, when one may introduce $\mu_{\text{eff}}=\mu/n$, where n is the number of polygons at the vertex (on the sphere) of a given type. As an example consider S(2, 3, 9)-scheme, when ($b=12$, $r=9$) for $\mu_{\text{eff}}=8$ and $n=3$ gives for $\mu=24$ a C_{72} (72-gon on the sphere). Furthermore, various types of decomposition of the given set into several subsets with their own characteristics (and the corresponding partition b), in particular, for the structures like the keplerates.

6. Conclusion

Prior to constructing systems involving non-crystallographic groups, we will briefly dwell on the local approach problem and the role of algebra in such constructions. The matter is that point or atom-generated varieties fall into totally disconnected ones by definition. Consequently, in the transition to local isomorphisms and discrete local groups, where there are algebraic operations to be performed in the neighborhood of group elements, natural difficulties emerge that can be settled in the context of an algebraic approach only. Indeed, such an approach permits linearising a whole series of problems through, for example, coordinatisation, when there is a correspondence between points (vectors) and their coordinates in that each type of variable is characterized by the law of its transformation. Note that transformations mapping a point space into itself are referred to as automorphisms and form a group (in the ordinary sense. The definition of a nanoparticle as a particle in which the numbers of surface and bulk atoms are comparable suggests that the nanoparticle can be constructed from a limited set of specific atomic groups of geometrical structural complexes. The joining of the geometrical structural complex to an elementary-similar cluster (embedded in the same algebraic construction) provides a way of assembling nanostructures with coherent boundaries.[17,18]

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