Tableau 8. *Groupe G_k associée à G*

G	Réseau	G_k	G	Réseau	G_k
$\bar{1}, m$	$3c$	1	$\bar{3}, 32$	$3a$	3
				$3c$	
2	$3a$	1		$3r, 3h$	
$2/m$	$3a$	m	$3m$	$3a$	3
	$3c$	$\bar{1}$			
222	$3c$	112	$\bar{3}m$		$3m$
$m_{yz}m_{zx}2$	$3a$	$1m1$	$\bar{6}$	$3c$	3
mmm	$3c$	2_zmm	6	$3a$	3
$\bar{4}$	$3c$	2	$6/m$	$3c$	6
				$3a$	$\bar{6}$
$422, 4/m$	$3c$	4			
			$\bar{6}2m$	$3c$	$3m$
$\bar{4}2m$	$3c$	$2mm$			
$4/mmm$	$3c$	$4mm$	$6mm$	$3a$	$3m$
			622	$3c$	6
				$3a$	32
			$6/mmm$	$3c$	$6mm$
				$3a$	$\bar{6}2m$

faut ici envisager les couples de représentations conjuguées, ou encore les groupes conjugués de chaque paire de Koptsik.

Les groupes G_{e3}^0 forment avec G_e un sous-groupe, les groupes G_{e3}^k ne forment pas un sous-groupe. On a:

$$G_{ek}^1 \times G_{e0}^3 = G_{ek}^3$$

$$G_{ek}^1 \times G_{ek'}^1 = G_{ek+k'}^1.$$

Par exemple: si $G_e = P6_3$, le groupe est formé de G_e, des groupes G_{e0}^3 colorés, ($P6_3^{(3)}$ et son conjugué $P6_3^{(3')}$) enfin, des trois groupes G_{ek}^i mentionnés plus haut et de leurs conjugués.

(b) Les groupes G_{e0}^i de classe isomorphe de G forment un groupe abélien additif dont l'unité est le groupe symmorphique $T_A G$. Ainsi:

$$P6_3^{(3)} + P6_3^{(3')} = P6^{(3)}.$$

les groupes G_{ek}^1 de réseau T_3 et de classe isomorphe à G forment un groupe dont l'unité est le groupe symmorphique $T_{3A}G$. Par exemple:

$$P_{3c}ma2 + P_{3c}bm2 = P_{3c}ba2.$$

Enfin, les groupes G_{ek}^i de réseau T_3 et de classe isomorphe à G forment un groupe plus large que le précédent. Par exemple:

$$P_{3c}cc2 + P_{3c}mn2_1 = P_{3c}ca2_1.$$

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On Periodic and Non-periodic Space Fillings of $\mathbb{E}^m$ Obtained by Projection

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Abstract

A periodic lattice in $\mathbb{E}^n$ is associated with an n-grid and its dual, and with a point symmetry group G. Given a subgroup H of G, a subspace $\mathbb{E}^m$, $m < n$, of $\mathbb{E}^n$, invariant under H, is chosen and a projection of the n-grid from $\mathbb{E}^n$ to $\mathbb{E}^m$ is defined. The translational and point symmetries of the projected n-grid are analyzed. A projection of the cubic n-grid from $\mathbb{E}^n$ to $\mathbb{E}^{n-1}$ based on $H = S(n)$ yields a periodic n-grid. A projection of the cubic 12-grid from $\mathbb{E}^{12}$ to $\mathbb{E}^3$ based on $H = A(5)$ yields a non-periodic 12-grid. This 12-grid is characterized by three real numbers and from its projection has a well defined orientation. The dual

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to this 12-grid yields a generalization of the non-periodic Penrose patterns from two to three dimensions.

1. Introduction

Penrose (1979) introduced non-periodic patterns in $\mathbb{E}^2$ in terms of two cells. de Bruijn (1981) developed an algebraic approach to these patterns. He introduced a pentagrid in $\mathbb{E}^2$ depending on two real numbers and showed that there is a one-to-one correspondence between Penrose patterns and dual graphs to the pentagrids. de Bruijn gave an algebraic description of the orientation for the graphs. Moreover, he showed that the pentagrid could be considered as the projection of a five-dimensional cubic cell structure from $\mathbb{E}^5$ to $\mathbb{E}^2$.

In the present paper we generalize several ideas of de Bruijn and study various applications. We introduce a projection of an n-grid Y in $\mathbb{E}^n$ to an n-grid Y_1 in $\mathbb{E}_1^m$, $1 \le m < n$. For the projection we consider the translation group T and the point group G of the original n-grid. We choose a subgroup $H < G$ and take the subspace $\mathbb{E}_1^m$ as a representation space of H. Then we project the n-grid Y onto $\mathbb{E}_1^m$ and investigate its symmetry under translation subgroups of T and point subgroups of H. With the projected n-grid Y_1 in $\mathbb{E}_1^m$ we associate a directed dual graph Z_1 which gives rise to a dual space filling of $\mathbb{E}^m$. In contrast to de Bruijn, we define the orientation of Z_1 through the projection procedure.

As a first example we project the cubic n-grid from $\mathbb{E}^n$ to $\mathbb{E}^{n-1}$ by use of the symmetric subgroup $H = S(n)$ of the hyperoctahedral point group $\Omega(n)$. We obtain a periodic n-grid Y_1 and dual graph Z_1 in $\mathbb{E}_1^{n-1}$ and consider in more detail the cases $n = 3$ and $n = 4$.

As the second example we project the cubic 12-grid from $\mathbb{E}^{12}$ to $\mathbb{E}^3$ by use of the icosahedral group $A(5)$ considered as a subgroup of $\Omega(12)$. We obtain a 12-grid Y_1 in $\mathbb{E}_1^3$, which is associated with the regular dodecahedron, is determined by three real numbers and is shown to have no translational subsymmetry. The dual graph Z_1 yields a space filling of $\mathbb{E}^3$ by two types of rhombohedral cells with directed edges. The cells coincide with the ones introduced by Mackay (1981) as a generalization of the Penrose pattern to three dimensions.

By the projection method we establish the association of the three-dimensional Penrose pattern with the icosahedral group and introduce an algebraic approach to this pattern based on the dual 12-grid. For a different association of the icosahedral group to non-periodic space filling of $\mathbb{E}^3$ we refer to Kramer (1982).

2. Grids, cells and graphs in $\mathbb{E}^n$

Let $\mathbb{E}^n$ be the real Euclidean vector space with the standard inner product, and let $\mathbf{b}_1\mathbf{b}_2\dots\mathbf{b}_n$ denote a basis of $\mathbb{E}^n$. We use the same symbol $\mathbb{E}^n$ to denote the set of points of the Euclidean space associated with this vector space.

2.1. *Definition*: An n-grid Y consists of n systems Y^i of hyperplanes

$$Y^i = \{\mathbf{y}|\mathbf{y}\,.\,\mathbf{b}_i = \tfrac{1}{2}k_i,\ k_i = \pm 1, \pm 3, \pm 5, \dots\},\quad i = 1, 2, \dots, n.$$

For fixed i, these hyperplanes are parallel and have as distances the multiples of $|\mathbf{b}_i|^{-1}$. The vectors $\mathbf{b}_i$ give a natural orientation to all systems Y^i.

2.2. *Definition*: The primitive translation cell of the n-grid Y with index system $(k_1k_2\dots k_n)$ is the set of points

$$\{\mathbf{y}|\tfrac{1}{2}(k_i - 2) < \mathbf{y}\,.\,\mathbf{b}_i \le \tfrac{1}{2}k_i,\ i = 1, 2, \dots, n\}$$

Since the cells do not overlap and fill all of $\mathbb{E}^n$, the index system defines n functions $k_i(P)$ for all points P of $\mathbb{E}^n$.

2.3. *Definition*: Choose a fixed point of $\mathbb{E}^n$ corresponding to the vector $\boldsymbol{\gamma}$ and write $\mathbf{y} = \boldsymbol{\gamma} + \mathbf{x}$. Then the n-grid Y referred to the point $\boldsymbol{\gamma}$ is given by the n systems of hyperplanes

$$Y^i = \{\mathbf{x}|\mathbf{x}\,.\,\mathbf{b}_i = \tfrac{1}{2}k_i - \boldsymbol{\gamma}\,.\,\mathbf{b}_i,\ k_i = \pm 1, \pm 3, \pm 5, \dots\},\quad i = 1, 2, \dots n.$$

2.4. *Definition*: The dual lattice to Y is the discrete set of points

$$\left\{\mathbf{k}\,\middle|\,\mathbf{k} = \tfrac{1}{2}\sum_{i=1}^{n} k_i\mathbf{b}_i,\ (k_1k_2\dots k_n) \text{ a cell index of } Y\right\}.$$

2.5. *Definition*: The dual graph Z to Y is a graph whose vertices are the points of the dual lattice and whose directed edges are given by connecting vertices $\mathbf{k}'$, $\mathbf{k}''$ which obey

$$\mathbf{k}' - \mathbf{k}'' = \sum_{i=1}^{n} \delta_{ji}\mathbf{b}_i \quad \text{for some } j,\ 1 \le j \le n.$$

2.6. *Definition*: The reciprocal basis $\mathbf{b}_1^*\mathbf{b}_2^*\dots\mathbf{b}_n^*$ to the basis $\mathbf{b}_1\mathbf{b}_2\dots\mathbf{b}_n$ is defined by the conditions $\mathbf{b}_i^*\,.\,\mathbf{b}_j = \delta_{ij}$.

We now describe the translation symmetries of the n-grid Y and its dual graph.

2.7. *Definition*: The translational group T is the group with elements

$$T = \left\{\mathbf{t}\,\middle|\,\mathbf{t} = \sum_{i=1}^{n} t_i\mathbf{b}_i^*,\ t_i = 0, \pm 1, \pm 2, \dots\right\},$$

the translation group T^* is the group with elements

$$T^* = \left\{\mathbf{h}\,\middle|\,\mathbf{h} = \sum_{i=1}^{n} h_i\mathbf{b}_i,\ h_i = 0, \pm 1, \pm 2, \dots\right\}.$$

2.8. *Proposition*: The n-grid Y is transformed into itself under the translation group T, the dual graph Z is transformed into itself under the translation group T^*.

Note that the dual graph has the interpretation of the graph of the group T^* with the directed edges being the n generators of T^*, *cf.* Grossman & Magnus (1964).

3. Projection of grids and graphs onto an orthogonal subspace

Consider an orthogonal decomposition of the vector space E^n,

$$E^n = E_1^m + E_2^{n-m},\ E_1^m \perp E_2^{n-m},\ 1 \le m < n.$$

By the indices 1 and 2 we denote the two orthogonal subspaces and the projection of any vector into these subspaces. We choose a fixed point corresponding to the vector $\boldsymbol{\gamma}$ and demand that it belongs to the subspace E_1^m.

3.1. *Definition*: The projected n-grid Y_1 in E_1^m is the set of points

$$Y_1^i = \{\mathbf{x} | \mathbf{x} \in Y^i \cap E_1^m\},\ i = 1, 2, \ldots, n.$$

The points of Y_1 are characterized by the conditions

$$\mathbf{x} \cdot \mathbf{b}_{i1} = \tfrac{1}{2}k_i - \boldsymbol{\gamma} \cdot \mathbf{b}_i,$$
$$k_i = \pm 1, \pm 3, \pm 5, \ldots, i = 1, 2, \ldots n.$$

Note that the projection depends on the choice of the point corresponding to $\boldsymbol{\gamma}$.

The projected n-grid Y_1 yields a division of E_1^m into cells according to

$$\{\mathbf{x} | \tfrac{1}{2}(k_i - 2) < \mathbf{x} \cdot \mathbf{b}_{i1} + \boldsymbol{\gamma} \cdot \mathbf{b}_i \le \tfrac{1}{2}k_i,\ i = 1, 2, \ldots, n\}.$$

Since any point P_1 of E_1^m belongs to precisely one cell, the index system $(k_1 k_2 \ldots k_n)$ defines again n functions $k_i(P_1)$ for all points P_1 of E_1^m. Because of the projection from E^n to E_1^m, the range of these functions is smaller than the one of the functions mentioned after Definition 2.2.

3.2. *Definition*: The dual lattice to the projected grid Y_1 is the discrete set of points

$$\left\{\mathbf{k} \,\middle|\, \mathbf{k} = \tfrac{1}{2} \sum_{i=1}^{n} k_i \mathbf{b}_{i1},\ (k_1 k_2 \ldots k_n) \text{ a cell index of } Y_1\right\}.$$

3.3. *Definition*: The dual graph Z_1 to Y_1 is the graph whose vertices are the points of the dual lattice and whose directed edges are given by connecting vertices $\mathbf{k}', \mathbf{k}''$ which obey

$$\mathbf{k}' - \mathbf{k}'' = \sum_{i=1}^{n} \delta_{ji} \mathbf{b}_{i1} \quad \text{for some } j,\ 1 \le j \le n.$$

Any finite cell of Y_1 has at least $m+1$ hyperplanar faces. At any face, the index of the neighbouring cells jumps by ± 2 in a single index. The edges of Z_1 correspond to the cell faces of Y_1, and hence it follows that at least $m+1$ directed edges meet at a vertex of the dual graph Z_1.

An edge of a cell of Y_1 is part of an intersection of m hyperplanes and joins $2m$ faces of cells. The $2m$ edges of Z_1 belonging to this edge form a closed subgraph and define a face of a cell structure belonging to Z_1. The vertices of Y_1 correspond to the cells of Z_1, and one sees that the graph Z_1 determines a dual space filling of E^m.

4. Translational symmetry under projection

We now inquire about the translational symmetry of Y and Z under projection. We restrict the attention to those translational symmetries of Y_1 and Z_1 which are subsymmetries of the groups T and T^*, respectively. This excludes accidental translational symmetries of Y_1 and Z_1 which have no counterpart in E^n.

4.1. *Proposition*: The projected n-grid Y_1 has a translational subsymmetry if and only if there exists an element $\mathbf{t}$ of T such that

$$\mathbf{t}_2 = \sum_{i=1}^{n} t_i \mathbf{b}_{i2}^* = 0, \qquad \sum_{i=1}^{n} (t_i)^2 > 0.$$

Proof: We rewrite the equations for the projected n-grid Y_1 in the equivalent form

$$\mathbf{x}_1 \cdot \mathbf{b}_i = \tfrac{1}{2}k_i - \boldsymbol{\gamma} \cdot \mathbf{b}_i.$$

Clearly, the projected n-grid is transformed into itself by any transformation $\mathbf{x}_1 \to \mathbf{x}_1 + \mathbf{t}$, $\mathbf{t} \in T$. If $\mathbf{t}_2 = 0$ then $\mathbf{t} = \mathbf{t}_1$ and hence the transformation is a translation $E_1^m \to E_1^m$, hence a subsymmetry. Conversely, assume that there exists a vector $\mathbf{v}_1 \in E_1^m, \mathbf{v}_1 \neq 0$ such that

$$\mathbf{x}_1 \cdot \mathbf{b}_i = \tfrac{1}{2}k_i - \boldsymbol{\gamma} \cdot \mathbf{b}_i, \quad i = 1, 2, \ldots, n,$$

implies

$$(\mathbf{x}_1 + \mathbf{v}_1) \cdot \mathbf{b}_i = \tfrac{1}{2}k_i' - \boldsymbol{\gamma} \cdot \mathbf{b}_i, \quad i = 1, 2, \ldots, n.$$

Then it follows that $\mathbf{v}_1 \cdot \mathbf{b}_i = \tfrac{1}{2}(k_i' - k_i) = \lambda_i = \text{integer}$. The vector

$$\mathbf{t} = \sum_{i=1}^{n} \lambda_i \mathbf{b}_i^*$$

clearly is an element of T and transforms Y_1 into itself. If we require $\mathbf{v}_1 \in T$ this implies $\mathbf{v}_1 = \mathbf{t} = \mathbf{t}_1$ and hence $\mathbf{t}_2 = 0$, $\mathbf{t}_1 \neq 0$.

4.2. *Proposition*: If the projected n-grid Y_1 has the translational subsymmetry group $T_1 < T$,

$$T_1 = \left\{\mathbf{t} \,\middle|\, \mathbf{t} = \sum_{i=1}^{n} t_i \mathbf{b}_{i1}^*\right\},$$

then the dual graph Z_1 has the translational symmetry group $T_1^* < T^*$,

$$T_1^* = \left\{ \mathbf{h} \middle| \mathbf{h} = \sum_{i=1}^{n} t_i \mathbf{b}_{i1} \right\}.$$

Note that the existence of a translational subsymmetry is independent of the choice of the vector $\boldsymbol{\gamma}$.

5. Point symmetry and projection

Let G denote the point symmetry group for the n-grid Y in E^n and consider a subgroup $H < G$. The action of G on E^n yields an n-dimensional orthogonal representation $G \to D$ which under subduction to H will in general be reducible. Assume that this representation of H has a direct sum decomposition

$$H: D \to D_1 + D_2$$

into two orthogonal representations D_1 and D_2 of dimensions m and $n - m$, respectively. Then the corresponding orthogonal subspaces E_1^m and E_2^{n-m} may be used to define the projection of the n-grid Y to the n-grid Y_1 in E_1^m. By this construction, the subgroup H of G acts within E_1^m and allows one to study the point symmetry group of the projected n-grid and its dual graph. Note that for a general choice of the point corresponding to $\boldsymbol{\gamma}$ the projected n-grid Y_1 does not have the point symmetry group H. If $\boldsymbol{\gamma}$ is decomposed as

$$\boldsymbol{\gamma} = \boldsymbol{\gamma}_1 + \boldsymbol{\gamma}_2,$$

a change of $\boldsymbol{\gamma}_1$ corresponds to a translational shift of the n-grid Y_1 and hence does not change its symmetry. It follows that the point symmetry group of Y_1 and of Z_1 depends on the vector $\boldsymbol{\gamma}_2$. We shall consider this result in the explicit constructions of §§ 6 and 7.

Strictly speaking, one should distinguish between the point symmetry groups of the n-grid and of the oriented n-grid. This distinction will be clear for the following examples.

6. Projection of the cubic n-grid from E^n to E^{n-1} based on the symmetric group $S(n)$

The cubic n-grid Y in E^n is defined through the orthonormal basis

$$\mathbf{b}_i : \mathbf{b}_i \cdot \mathbf{b}_j = \delta_{ij},\ i, j = 1, 2, \ldots, n.$$

The hyperplanes Y^i divide E^n into cubic cells. The dual lattice is again cubic, the dual graph Z has the directed edges of the cubes as its elements. The reciprocal basis $\mathbf{b}_i$ coincides with $\mathbf{b}_i^*$, and the translation groups T^* and T are isomorphic.

The point group G of the cubic n-grid is the hyperoctahedral group $\Omega(n)$. This group contains the subgroup $S(n)$ of all permutations of the n basis vectors along with n reflections of the type $\mathbf{b}_i \to -\mathbf{b}_i$. We choose the subgroup $H = S(n)$ of $\Omega(n)$ for the projection. The representation D of $S(n)$ has the decomposition

$$S(n): D \to D_1^{n-1} + D_2^1,$$

where D_1 corresponds to the Young diagram $[n-11]$ and D_2 corresponds to the Young diagram $[n]$, respectively. The projection of the basis into the corresponding subspaces E_1^{n-1} and E_2^1 is easily found to be

$$\mathbf{b}_{i1} = \mathbf{b}_i - \frac{1}{n} \sum_{j=1}^{n} \mathbf{b}_j, \qquad \mathbf{b}_{i2} = \frac{1}{n} \sum_{j=1}^{n} \mathbf{b}_j.$$

The projected basis vectors in E_1^{n-1} have the scalar products

$$\mathbf{b}_{i1} \cdot \mathbf{b}_{j1} = \delta_{ij} - 1/n,$$

and from this one finds

$$|\mathbf{b}_{i1}| = [(n-1)/n]^{1/2},$$

$$\cos(\mathbf{b}_{i1}, \mathbf{b}_{j1}) = -(n-1)^{-1}, \quad i \neq j.$$

To find the translational subsymmetry group T_1 we apply proposition 4.1,

$$T_1 = \left\{ \mathbf{h} \middle| \mathbf{h} = \sum_{i=1}^{n} t_i \mathbf{b}_{i1},\ \sum_{j=1}^{n} t_j = 0 \right\}.$$

The n-grid Y_1 depends on the numbers $\boldsymbol{\gamma} \cdot \mathbf{b}_i$. We decompose $\boldsymbol{\gamma}$ as

$$\boldsymbol{\gamma} = \boldsymbol{\gamma}_1 + \boldsymbol{\gamma}_2.$$

By a translational shift in E_1^{n-1} we can change $\boldsymbol{\gamma}_1$ without changing the intrinsic structure of Y_1. Putting for example $\boldsymbol{\gamma}_1 = 0$, we get

$$\boldsymbol{\gamma} \cdot \mathbf{b}_i = \boldsymbol{\gamma}_2 \cdot \mathbf{b}_{i2} = \gamma$$

so that the n-grid Y_1 is determined by a single number γ. Consider now the vertices of the n-grid Y_1, that is, the intersection points of the n systems of hyperplanes. We call an intersection point regular if at most $n-1$ hyperplanes intersect, otherwise singular.

6.1. *Proposition*: The projected n-grid Y_1 in E_1^{n-1} is determined by a single real number γ. All vertices of Y_1 are singular for the discrete values

$$\gamma = n^{-1} \tfrac{1}{2} k, \quad k = \begin{cases} 0, \pm 2, \pm 4, \ldots \text{ for } n \text{ even} \\ \pm 1, \pm 3, \pm 5, \ldots \text{ for } n \text{ odd}, \end{cases}$$

otherwise all vertices are regular.

Proof: Without loss of generality we may study an intersection point belonging to the systems $Y_1^1 Y_1^2 \ldots Y_1^{n-1}$ of hyperplanes and fixed values $k_1 k_2 \ldots k_{n-1}$,

$$\mathbf{x} \cdot \mathbf{b}_{i1} = \tfrac{1}{2} k_i - \gamma, \quad i = 1, 2, \ldots, n-1.$$

Using $\sum_{j=1}^{n} \mathbf{b}_{j1} = 0$ this implies

$$\mathbf{x} \cdot \mathbf{b}_{n1} = -\tfrac{1}{2} \sum_{j=1}^{n-1} k_j + (n-1)\gamma.$$

From the values taken by the numbers k_i, the point lies in a hyperplane of the system Y_1^n with index k_n if

$$n\gamma = \tfrac{1}{2}k,$$

$$k = \sum_{j=1}^{n-1} k_j + k_n = \begin{cases} 0, \pm 2, \pm 4, \dots \text{ for } n \text{ even} \\ \pm 1, \pm 3, \pm 5, \dots \text{ for } n \text{ odd.} \end{cases}$$

Conversely, assume that γ has a value as stated in the proposition. Then for any intersection point of the first $n-1$ systems of hyperplanes one gets

$$\mathbf{x}\,.\,\mathbf{b}_{n1} = -\tfrac{1}{2}\sum_{j=1}^{n-1} k_j + \tfrac{1}{2}k - \gamma$$

$$= \tfrac{1}{2}k_n' - \gamma, \quad k_n' = -\sum_{j=1}^{n-1} k_j + k = \pm 1, \pm 3, \dots$$

and hence all intersection points are singular.

Example 1: *Projection of the cubic* 3-*grid from* E^3 *to* E^2. In this case the three projected vectors $\mathbf{b}_{i1}$ have the properties

$$|\mathbf{b}_{i1}| = (2/3)^{1/2}, \qquad \cos(\mathbf{b}_{i1}, \mathbf{b}_{j1}) = -\tfrac{1}{2} \quad \text{for } i \neq j.$$

The translation subgroup is

$$T_1 = \left\{ \mathbf{h} \,\middle|\, \mathbf{h} = \sum_{i=1}^{3} t_i \mathbf{b}_{i1},\ t_1 + t_2 + t_3 = 0 \right\}.$$

The point subgroup of Y_1 is the group C_{3v} isomorphic to $S(3)$. In Figs. 1 and 2 we show the 3-grid Y_1 for the regular and the singular cases. In the singular case we have

$$\gamma = \tfrac{1}{3}\tfrac{1}{2}k, \qquad k = \pm 1, \pm 3, \dots.$$

The vertices of Y_1 determine the cells for the dual graph Z_1. For regular vertices, the cells of Z_1 are of rhombus shape with a fixed orientation shown in Fig. 3. For singular vertices of Y_1, the cells of Z_1 are regular hexagons with a definite orientation, see Fig. 4.

Example 2: *Projection of the cubic* 4-*grid from* E^4 *to* E^3. The projected vectors in E^3 have the properties

$$|\mathbf{b}_{i1}| = (3/4)^{1/2}, \qquad \cos(\mathbf{b}_{i1}, \mathbf{b}_{j1}) = -1/3 \quad \text{for } i \neq j,$$

they are perpendicular to the faces of the regular tetrahedron. The translation group T_1 has the general form given above, the point symmetry group of Y_1 is the tetrahedral group T_d isomorphic to $S(4)$. We now describe the structure of Y_1 and Z_1 and put in brackets the generalization of the description to the general case.

An edge of a cell of Y_1 belongs to the intersection of four $[2(n-2)]$ faces of cells. A regular vertex of Y_1 belongs to six $[2(n-1)]$ edges, a singular vertex of Y_1 belongs to 12 $[n(n-1)]$ edges. The dual structure of Z_1 has the following features: To a face of a cell of Y_1 there corresponds a directed vertex of Z_1. The four $[2(n-2)]$ faces of Y_1 meeting at an edge of Y_1 give rise to a closed connected part of Z_1 which we call a (hyper-)rhombus. This (hyper-)rhombus lies in the (hyper-)plane perpendicular to the edge of Y_1 and contains four $[2(n-2)]$ vectors $\mathbf{b}_{i1}$ which appear twice. To a vertex of Y_1 there corresponds a cell Z_1. For a regular vertex, the cell of Z_1 has six $[2(n-1)]$ (hyper-)rhombus faces and forms an oriented (hyper-)rhombohedron. For a singular vertex of Y_1, the cell of Z_1 has 12 $[n(n-1)]$ (hyper-)rhombus faces.

We do not discuss the cell structure of Y_1 which corresponds to the vertex structure of Z_1.

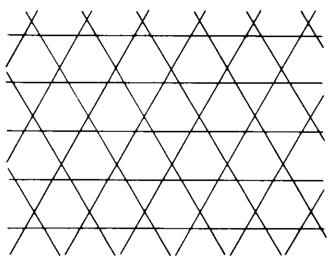

Fig. 1. Projection of the cubic 3-grid from E^3 to E^2 in the regular case.

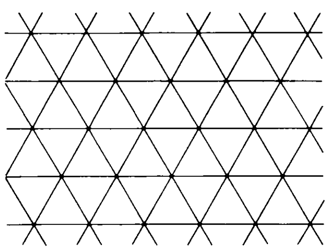

Fig. 2. Projection of the cubic 3-grid from E^3 to E^2 in the singular case.

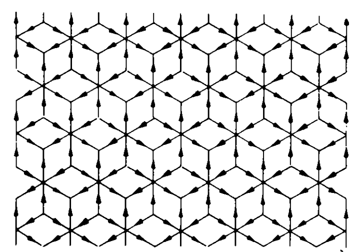

Fig. 3. The dual directed graph and space filling for the regular projected 3-grid.

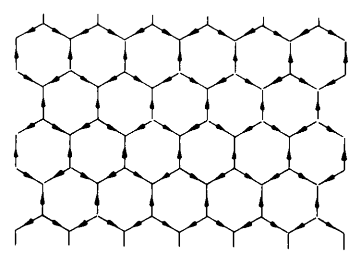

Fig. 4. The dual directed graph and space filling for the singular projected 3-grid.

Table 1. *Generators g_2 and g_5 of order 2 and 5 for the icosahedral group $A(5)$ taken as a subgroup of $S(12)$*

$$g_2: \begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 \\ 3 & 6 & 1 & 9 & 8 & 2 & 11 & 5 & 4 & 12 & 7 & 10 \end{bmatrix}$$

$$g_5: \begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 \\ 2 & 3 & 4 & 5 & 1 & 6 & 7 & 12 & 8 & 9 & 10 & 11 \end{bmatrix}$$

Table 2. *Representation $D_{1'}$ and $D_{2'}$ of $A(5)$ in the bases $\mathbf{c}_i$, $i=1,2,\ldots,6$, and $\mathbf{c}_{i+6}$, $i=1,2,\ldots,6$, respectively, for the generators g_2 and g_5*

The upper sign applies to $D_{1'}$, the lower sign to $D_{2'}$.

$$g_2: \begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 3 & 6 & 1 & \mp 4 & \mp 5 & 2 \end{bmatrix}$$

$$g_5: \begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 2 & 3 & 4 & 5 & 1 & 6 \end{bmatrix}$$

7. Projection of the cubic 12-grid from $\mathbb{E}^{12}$ to $\mathbb{E}^3$ based on the icosahedral group $A(5)$

The cubic 12-grid in $\mathbb{E}^{12}$ has the point symmetry group $\Omega(12)$ with the subgroup $S(12)$. Consider the subgroup $C(5)$ of $A(5)$, the cyclic group. The group $A(5)$ acts on the 12 cosets $A(5)/C(5)$ as a permutation group of 12 objects and therefore yields an embedding $A(5) < S(12) < \Omega(12)$. If the icosahedral rotations of the regular dodecahedron are interpreted as permutations of the twelve faces, we obtain the explicit form of this embedding. The enumeration of the dodecahedral faces is taken from Kramer (1982) and leads to Table 1.

The representation D of $S(12)$ in $\mathbb{E}^{12}$ is given by the standard permutation matrices. For the subduction to a representation of $A(5)$ we note that the generators g_2 and g_5 have been chosen with the following property: If $p \in A(5)$ sends i into $p(i) = j$, then $p(13-i) = 13-j$. Now we pass from the basis $\mathbf{b}_1\mathbf{b}_2 \ldots \mathbf{b}_n$ to the new basis

$$\begin{aligned} \mathbf{c}_i &= (1/2)^{1/2}(\mathbf{b}_i - \mathbf{b}_{13-i}) \\ \mathbf{c}_{i+6} &= (1/2)^{1/2}(\mathbf{b}_i + \mathbf{b}_{13-i}) \end{aligned} \quad i = 1, 2, \ldots, 6.$$

In this new basis, the representation D subduced to $A(5)$ decomposes into two six-dimensional representations $D_{1'}$ and $D_{2'}$ specified in Table 2.

For the irreducible representations of $A(5)$ we use a notation based on the symmetric group $S(5)$ and its subduction to $A(5)$, Table 3. The representations may be identified by their characters, Table 4.

By standard methods one finds the decompositions of $D_{1'}$ and $D_{2'}$ under $A(5)$:

$$\begin{aligned} D_{1'} &= D^{[311]^i} + D^{[311]^\omega} \\ D_{2'} &= D^{[32]} + D^{[5]}. \end{aligned}$$

By character projection technique one constructs the explicit reduction of the representation $D_{1'}$.

Table 3. *Subduction of irreducible representations from $S(5)$ to $A(5)$*

$S(5)$	Dimension	$A(5)$	Dimension
[5]	1	[5]	1
[11111]	1	[11111]~[5]	
[41]	4	[41]	4
[2111]	4	[2111]~[41]	
[32]	5	[32]	5
[221]	5	[221]~[32]	
[311]	6	$[311]^i + [311]^\omega$	
		$[311]^i$	3
		$[311]^\omega$	3

Table 4. *Characters χ for irreducible representations of $A(5)$*

Class representatives are the identity element e, powers of the generators g_2 and g_5, and the elements of order 3 derived from $g_3 = g_2 g_5$. The number ϕ is $\phi = (1 + 5^{1/2})/2$.

Class representative	Number of elements	Irreducible representation				
		[5]	[41]	[32]	$[311]^i$	$[311]^\omega$
e	1	1	4	5	3	3
g_2	15	1	0	1	-1	-1
g_3^2, g_3^2	20	1	1	-1	0	0
g_5, g_5^4	12	1	-1	0	ϕ	$1-\phi$
g_5^2, g_5^3	12	1	-1	0	$1-\phi$	ϕ

7.1. *Proposition*: In the new basis of $\mathbb{E}^6_{1'}$ for $D_{1'}$ defined by

$$\mathbf{d}_i = \sum_{j=1}^{6} m_{ij}\mathbf{c}_j, \quad i = 1, 2, \ldots, 6$$

and the matrix m given by

m	1	2	3	4	5	6
1	$(1/10)^{1/2}$	$(1/10)^{1/2}$	$(1/10)^{1/2}$	$(1/10)^{1/2}$	$(1/10)^{1/2}$	$(1/2)^{1/2}$
2	$(2/5)^{1/2}$	$(2/5)^{1/2}c$	$(2/5)^{1/2}c'$	$(2/5)^{1/2}c'$	$(2/5)^{1/2}c$	0
3	0	$-(2/5)^{1/2}s$	$-(2/5)^{1/2}s'$	$(2/5)^{1/2}s'$	$(2/5)^{1/2}s$	0
4	$-(1/10)^{1/2}$	$-(1/10)^{1/2}$	$-(1/10)^{1/2}$	$-(1/10)^{1/2}$	$-(1/10)^{1/2}$	$(1/2)^{1/2}$
5	$(2/5)^{1/2}$	$(2/5)^{1/2}c'$	$(2/5)^{1/2}c$	$(2/5)^{1/2}c$	$(2/5)^{1/2}c'$	0
6	0	$-(2/5)^{1/2}s'$	$(2/5)^{1/2}s$	$-(2/5)^{1/2}s$	$(2/5)^{1/2}s'$	0

where $c = \cos 2\pi/5$, $s = \sin 2\pi/5$, $c' = \cos 4\pi/5$, $s' = \sin 4\pi/5$, the representation $D_{1'}$ is explicity reduced as

$$D_{1'} = m \begin{bmatrix} D_1 & 0 \\ 0 & D_2 \end{bmatrix} m^{-1}, \quad D_1 = D^{[311]^i}, \quad D_2 = D^{[311]^\omega}.$$

Now we project in a first step the cubic 12-grid from $\mathbb{E}^{12}$ to the subspace $\mathbb{E}^6_{1'}$ determined by the reducible representation $D_{1'}$ of $A(5)$. Inverting the relation between the bases $\mathbf{b}_i$ and $\mathbf{c}_i$ introduced above we get

$$\begin{aligned} \mathbf{b}_{i,1} &= (1/2)^{1/2}\mathbf{c}_i \quad & i = 1, 2, \ldots, 6 \\ \mathbf{b}_{13-i,1} &= -(1/2)^{1/2}\mathbf{c}_i \quad & i = 1, 2, \ldots, 6 \end{aligned}$$

and the projected 12-grid in $\mathbb{E}^6_{1'}$ has the equations

$$\begin{aligned} \mathbf{x} \cdot \mathbf{b}_{i,1} &= \tfrac{1}{2}k_i - \boldsymbol{\gamma} \cdot \mathbf{b}_i, \quad & i = 1, 2, \ldots, 6, \\ \mathbf{x} \cdot \mathbf{b}_{13-i,1} &= \tfrac{1}{2}k_{13-i} - \boldsymbol{\gamma} \cdot \mathbf{b}_{13-i}, \quad & i = 1, 2, \ldots, 6. \end{aligned}$$

For fixed i, the systems Y^i_1 and Y^{13-i}_1 of hyperplanes in $E^6_{1'}$ are parallel but have opposite orientation. Now we choose in $E^6_{2'}$

$$\gamma_{2'} \cdot \mathbf{b}_i = \gamma_{2'} \cdot \mathbf{b}_{13-i} = \tfrac{1}{4}.$$

This choice of γ allows one to describe the 12-grid in $E^6_{1'}$ by the set of equations

$$\mathbf{x} \cdot \mathbf{c}_i = \tfrac{1}{4} 2^{1/2} \tau_i - \gamma_{1'} \cdot \mathbf{c}_i, \ \tau_i = \pm 1, \pm 3, \pm 5, \ldots, \quad i = 1, 2, \ldots, 6,$$

where all hyperplanes for $\tau_i = 1, -3, 5, \ldots$ have the orientation determined by $\mathbf{c}_i$ and for $\tau_i = -1, 3, -5, \ldots$ have the orientation determined by $-\mathbf{c}_i$. The 12-grid in $E^6_{1'}$ becomes a cubic 6-grid with alternating orientation of parallel hyperplanes.

In the second step we project this modified 6-grid from $E^6_{1'}$ to E^3_1, the representation space of the irreducible representation $D^{[311]'}$ of $A(5)$. Using the orthogonal matrix m one finds, for the projections of the vectors $\mathbf{c}_i$,

$$\mathbf{c}_{i1} = \sum_{j=1}^{3} m_{ji} \mathbf{d}_j \qquad \mathbf{c}_{i2} = \sum_{j=4}^{6} m_{ji} \mathbf{d}_j$$

with

$$|\mathbf{c}_{i1}| = |\mathbf{c}_{i2}| = (1/2)^{1/2}.$$

The equations for the projected 12-grid Y_1 in E^3_1 become

$$\mathbf{x} \cdot 2^{1/2} \mathbf{c}_{i1} = \tfrac{1}{2} \tau_i - \gamma_i, \quad \tau_i = \pm 1, \pm 3, \pm 5, \ldots$$
$$\gamma_i = 2^{1/2} \gamma_{1'} \cdot \mathbf{c}_i, \ i = 1, 2, \ldots, 6.$$

7.2. *Proposition*: The 12-grid of E^{12} under projection to the irreducible representation space E^3_1 of the representation $D^{[311]'}$ becomes a hexagrid whose planes are perpendicular to the twelve faces of the regular dodecahedron. The distance of consecutive parallel planes is 1, and these planes have alternating orientation.

Proof: The normalized vectors $(2)^{1/2} \mathbf{c}_{i1}$ are obtained from the six columns of the matrix $m = (m_{ij})$ for $i = 1, 2, 3$. These vectors determine the directions perpendicular to the faces of the regular dodecahedron. The orientation of the planes alternates according to the value of τ_i. This property reflects the existence of a 12-grid rather than a 6-grid.

7.3. *Proposition*: The projected 12-grid in E^3_1 has no translational subsymmetry of the translation group for the cubic 12-grid in E^{12}.

Proof: Firstly, we consider the projection from E^{12} to $E^6_{1'}$. The translation subgroup is easily found to be

$$T_{1'} = \left\{ \mathbf{t} \,\middle|\, \mathbf{t} = \sum_{i=1}^{12} t_i \mathbf{b}_{i1}, \ t_j + t_{13-j} = 0, \quad j = 1, 2, \ldots, 6 \right\}$$
$$= \left\{ \mathbf{t} \,\middle|\, \mathbf{t} = \sum_{i=1}^{6} t_i 2^{1/2} \mathbf{c}_i \right\}.$$

Clearly this translation subgroup maps the oriented hyperplanes of the 12-grid in $E^6_{1'}$ into one another. Now consider the projection from $E^6_{1'}$ to E^3_1. From proposition 3.1 we require a translation vector such that

$$\sum_{i=1}^{6} t_i \mathbf{c}_{i2} = 0, \qquad \sum_{i=1}^{6} (t_i)^2 > 0.$$

In terms of the matrix m, this condition becomes

$$\sum_{i=1}^{6} t_i m_{ji} = 0, \quad j = 4, 5, 6.$$

For $j = 4$, the equation reads

$$(10)^{-1/2} \sum_{i=1}^{5} t_i - (2)^{-1/2} t_6 = 0,$$

which for integer numbers t_i implies

$$\sum_{i=1}^{5} t_i = 0, \qquad t_6 = 0.$$

The operations of $A(5)$ allow one to replace the vector $\mathbf{c}_{62}$ by any other vector $\mathbf{c}_{j2}, j = 1, 2, \ldots, 5$. Therefore, all the integers t_i must be zero, and hence there is no translation subgroup.

We turn to a description of the projected 12-grid Y_1 and its dual Z_1. An edge of Y_1 is the intersection of two planes whose normal vectors form an angle φ with $\cos \varphi = \pm (1/5)^{1/2}$. A regular vertex of Y_1 is the intersection of three planes. There are two types of triples of planes: in the first case we may choose three normal vectors with the same angle φ, $\cos \varphi = (1/5)^{1/2}$, in the second case we may choose three normal vectors with the same angle φ', $\cos \varphi' = -(1/5)^{1/2}$. The edges of Y_1 determine the faces of Z_1. The face of Z_1 is a rhombus with the two angles characterized by $\cos \varphi = \pm (1/5)^{1/2}$. There are two possible orientations of the edges, see Fig. 5.

The cell of Z_1 dual to the regular vertices of Y_1 are rhombohedra. Their edges at the vertices with threefold symmetry form the two triples of vectors described above. The direction of parallel edges is always the same, otherwise all combinations of directions are possible. The two types of rhombohedra are

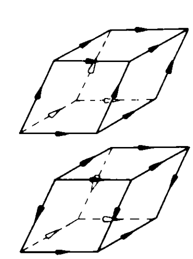

Fig. 5. The two possible orientations of the edges for one of the rhombohedra from Fig. 6.

shown in Fig. 6. The regular graph Z_1 describes a space filling of $\mathbb{E}^3$ by the two types of rhombohedra. This space filling has no translational subsymmetry from the cubic lattice in $\mathbb{E}^{12}$.

Finally, we note that a translation shift in $\mathbb{E}_1^3$ does not change Y_1 or Z_1 in their intrinsic structure. It follows that the 12-grid Y_1 and its dual Z_1 are determined by three real numbers.

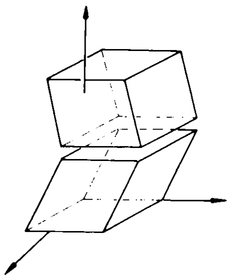

Fig. 6. Projection of the cubic 12-grid from $\mathbb{E}^{12}$ to $\mathbb{E}^3$. The cells of the dual space filling are two different types of rhombohedra.

As mentioned before, the two types of rhombohedra were introduced by Mackay (1981) as the cells for a generalization of the patterns introduced by Penrose (1979) from two to three dimensions. What we believe is new in the present approach is the projection from $\mathbb{E}^{12}$ to $\mathbb{E}^3$, the clear association with the icosahedral group $A(5)$, the introduction of the 12-grid and hexagrid in $\mathbb{E}^3$, and the treatment of the orientation for the grid and its dual.

The present projection method opens the way towards the complete geometric analysis and classification of the hexagrids and their duals.

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Shell Population and κ Refinements with Canonical and Density-Localized Scattering Factors in Analytical Form

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Abstract

Scattering factors for outer shells of the first- and second-row series of atoms have been obtained by expansions with Jacobi functions. Both canonical and density-localized shell form factors have been studied. For κ refinements, both first and second derivatives are computed by analytical methods. Density-localized shell distributions differ from canonical shell distributions within a small sphere (<0·5 Å) about the nucleus. Shell population and κ refinements on uracil at the monopole level give virtually identical results with canonical and density-localized form factors.

Introduction

In multipole analyses of electron density distributions from measured X-ray structure factors, the contraction o: expansion of the atoms due to chemical bonding and redistribution of charge is often considered. For the monopole this can be partly achieved by keeping the density functions of the shells of a spherically averaged Hartree–Fock atom fixed, but with variable populations in the respective shells. Moreover, in κ refinements (Coppens, Guru Row, Stevens, Becker & Yang, 1979) the outermost shell of each atom can be contracted or expanded by rescaling K ($4\pi \sin\theta/\lambda$) as K/κ, with κ as a variable. For $\kappa > 1$ the shell density is contracted and for $\kappa < 1$ it is expanded. The results of shell populations and κ scaling may depend on the partitioning of the IAM (independent atom model) density into shells. The usual practice is to take atomic shell functions based on canonical Hartree–Fock atomic orbitals. In this case the valence-shell density on the nucleus is non-zero. As an example, for N(^4S) the valence density is 64·4 e Å^3 compared to the core density of 1325·5 3 Å^3 on the nucleus. One can seek a unitary transformation of the 1s and 2s canonical orbitals that minimizes the overlap of the $(1s')^2$ and $(2s')^2$

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