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Crystallography, Geometry and Physics in Higher Dimensions. I. Point-Symmetry Operations

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Abstract

Physical phenomena such as incommensurate phases or diffraction enhancement of symmetry are interpreted by using symmetry groups in four, five or six dimensions. This first paper concerns the point-symmetry operations (PSO) in these Euclidean superspaces. Elementary, non-elementary, degenerate and non-degenerate PSOs are defined and their geometrical supports and geometrical symbols are specified. A geometrical description is thus given of nineteen types of PSO which are either the crystallographic rotations of the four-dimensional space or the crystallographic rotations and improper rotations of the five-dimensional space or the improper crystallographic rotations of the six-dimensional space. These PSOs are elements of crystallographic point groups of these spaces and the physical application to polar point groups is given.

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General introduction

Regularities observed in the diffraction pattern of a crystal and not explained by the three-dimensional Euclidean symmetry – called external space symmetry – are interpreted as due to Euclidean symmetry in a $(3+d)$-dimensional superspace involving d additional dimensions, called internal dimensions (Janner & Janssen 1980).

The following cases of incommensurate phases are well known; according to whether the incommensurability is parallel to a crystallographic direction, to a direction of a crystallographic plane or to any direction of the crystal, one, two or three additional (internal) d dimensions may be introduced (de Wolff, 1974; Comes, Lambert & Zeller, 1973; Janner & Janssen, 1977; Yamamoto, 1982).

The symmetry of diffraction patterns of some layered or intercalate crystals may be higher than that corresponding to the Friedel–Laue class (Sadanaga & Takeda, 1968; Marumo & Saito, 1972; Iwasaki, 1972). This phenomenon has been termed 'diffraction enhancement of symmetry' and two types – simple and double – have been analysed (Perez-Mato &

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Iglesias, 1977; Sadanaga & Ohsumi, 1979). If one uses a supercrystal in a $(3+d)$-dimensional superspace one finds that the experimental diffraction pattern has the Laue symmetry belonging to the external point group of the supergroup – *i.e.* the three-dimensional point group consisting of external components of the superspace group (Janner & Janssen, 1980).

So, it is important to study crystallography in four, five, six *etc.* dimensions and in particular its geometric and physical aspects: this is the purpose of this series of papers; the first papers treat the point symmetry and its possible physical applications.

Introduction

Point-symmetry operation (PSO) groups, in other words the isometric mappings of four-dimensional Euclidean space $\mathbb{E}^4$, have been studied from as far back as the end of the 19th century.

Goursat (1889) had already given a list classifying them into two families: the first is the set of all proper rotation groups which he called right substitution, the second is the set of all groups containing at least one improper rotation (or rotation–reflection) which he called left substitution.

As he studied the characteristic polynomial* of a point-symmetry operation in a space of n dimensions, Hermann (1949) enumerated various types of crystallographic PSO and proposed a notation for PSOs connected to their polynomial roots (eigenvalues).

Hurley (1951), following and implementing Goursat's works, drew up, in $\mathbb{E}^4$, the list of crystallographic groups and their elements (PSOs) for which he proposed also a notation connected to the characteristic polynomial invariants: one capital letter followed by values of the three invariants.

Neubüser, Wondratschek & Bülow (1971; Bülow, Neubüser & Wondratschek, 1971; Wondratschek, Bülow & Neubüser, 1971) utilized Hurley's (1951) symbols to describe elements of holohedric geometric crystal classes relative to the 33 crystal systems classified into 23 crystal families in $\mathbb{E}^4$.

None of these authors aimed at geometrically describing the various PSOs of $\mathbb{E}^n$. Throughout this paper, we define the elementary, non-elementary, degenerate and non-degenerate PSOs with the purpose of correctly describing for the first time their geometric supports: this leads us to give a very clear geometric notation for each type of PSO in $\mathbb{E}^4$, $\mathbb{E}^5$ and for a few of $\mathbb{E}^6$.

* Appendix 1 recalls the definitions of the characteristic polynomial and the eigenvalues of an isometry of $\mathbb{E}^n$, or more precisely of the orthogonal associated transform in $\mathbb{E}^n$.

I. Point-symmetry operations of $\mathbb{E}^n$

Throughout the following papers, $\mathbb{E}^n$ denotes a Euclidean vector space defined over the field of reals $\mathbb{R}$ and $\mathbb{E}^n$ denotes the corresponding affine space.

Definition. A point-symmetry operation (PSO) or point isometry is an intrinsic mapping of $\mathbb{E}^n$ leaving any distance or 'norm' and at least a point of $\mathbb{E}^n$ unchanged.

Each PSO is fully described by its eigenvalues associated with their multiplicity order. Let

q be the multiplicity of 1 eigenvalue;

r be the multiplicity of -1 eigenvalue;

s be the number of pairs of eigenvalues denoted $e^{i\theta}$ and $e^{-i\theta}$, $e^{i\varphi}$ and $e^{-i\varphi}, \ldots$, where $\theta, \varphi, \ldots$ belong to $[-\pi, 0] \cup [0, \pi]$.

It is clear that $q+r+2s=n$.

Eigenvalues $+1$ and -1 are associated with $\mathbb{E}^q$ and $\mathbb{E}^r$ eigenspaces, respectively. To each pair of eigenvalues $e^{i\theta}$ and $e^{-i\theta}$ corresponds a globally unchanged real plane $\mathbb{E}^2_\theta$ in which the isometry is reduced to a unique rotation of angle θ.

Then $\mathbb{E}^n$ admits a direct sum decomposition into two by two orthogonal eigenspaces:

$$\mathbb{E}^n = \mathbb{E}^q \oplus \mathbb{E}^r \oplus \mathbb{E}^2_\theta \oplus \mathbb{E}^2_\varphi \oplus \ldots \quad (1)$$

and this decomposition is unique if $\theta \neq \varphi \neq \psi \ldots$.

It is pointed out that the geometrical pattern of a PSO relies, on the one hand, on the vector spaces $\mathbb{E}^q$, $\mathbb{E}^r$ and the s planes $\mathbb{E}^2$ and, on the other hand, on the two numbers $+1$ and -1 and the values of the angles θ, φ, *etc.*

The point-symmetry operation is called a rotation denoted by OPS^+ if r is an even number and an inversion–rotation or reflection–rotation denoted by OPS^- if r is an odd number.

Extrinsic pattern of a PSO

Let $(e_1, \ldots, e_n)$ be an orthonormal basis of $\mathbb{E}^n$. In this basis the PSO is described by means of an orthogonal matrix* $A_\perp$ such that

$$X^{\cdot} = A_\perp X$$

where X and $X^{\cdot}$ denote the column matrices built with the n coordinates of the vector **OP** and its image **OP**$^{\cdot}$.

If the determinant value is equal to $+1$, the PSO is a PSO^+, if equal to -1 it is a PSO^-.

There exists at least one orthonormal 'reduction' basis among which the A matrix can be written as

* An orthogonal matrix has the following properties, with respect to an orthonormal basis: (1) ${}^tA_\perp = A_\perp^{-1}$; (2) $\det A_\perp = \pm 1$.

follows:

$$A = \begin{pmatrix} I_q & & & \\ & \bar{I}_r & & \\ & & \Delta\theta & \\ & & & \Delta\varphi \end{pmatrix} \quad (2)$$

with

$$\Delta\theta = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix},$$

where I_q denotes the identity matrix of $\mathbb{E}^q$, $\bar{I}_r$ the '*homothetie* −1' matrix* of $\mathbb{E}^r$, $\Delta\theta, \Delta\varphi, \ldots$ the rotation matrices of $\mathbb{E}^2_\theta, \mathbb{E}^2_\varphi, \ldots$. A 'reduction' basis is composed of orthonormal vectors of orthogonal bases of $\mathbb{E}^q, \mathbb{E}^r, \mathbb{E}^2, \mathbb{E}^2, \ldots$

Examples. Given the four orthogonal matrices in $\mathbb{E}^2, \mathbb{E}^3, \mathbb{E}^4, \mathbb{E}^5$:

$$(\Delta\theta) \quad \begin{pmatrix} 1 & \\ & \Delta\theta \end{pmatrix} \quad \begin{pmatrix} 1 & & \\ & 1 & \\ & & \Delta\theta \end{pmatrix} \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & \Delta\theta \end{pmatrix},$$

they represent PSOs that can be considered: either as rotations through the angle θ in $\mathbb{E}^2_{xy}$, $\mathbb{E}^2_{yz}$, $\mathbb{E}^2_{zt}$, $\mathbb{E}^2_{tu}$; or as a rotation through the angle θ about the point 0 of $\mathbb{E}^2$, about the axis x of $\mathbb{E}^3$, about the plane xy of $\mathbb{E}^4$, about the space xyz of $\mathbb{E}^5$.

We recall that in $\mathbb{E}^4$ the planes xy and zt meet only at the point 0 since $(\mathbf{x}, \mathbf{y}, \mathbf{z}, \mathbf{t})$ is a basis of $\mathbb{E}^4$.

Elementary PSOs of $\mathbb{E}^n$

Definition. Given the matrix (2), extrinsic writing of the most general PSO of $\mathbb{E}^n$; if $\theta \neq \varphi \neq \psi \neq \ldots \neq k\pi$, then there exists a unique decomposition of this matrix into a commutative product

$$\begin{pmatrix} I_q & & & & \\ & \bar{I}_r & & & \\ & & \Delta\theta & & \\ & & & \Delta\varphi & \\ & & & & \ddots \end{pmatrix} = \begin{pmatrix} 1 & & & & & & \\ & \ddots & & & & & \\ & & 1 & & & & \\ & & & \bar{I}_r & & & \\ & & & & 1 & & \\ & & & & & \ddots & \\ & & & & & & 1 \end{pmatrix}$$

$$\times \begin{pmatrix} 1 & & & & & \\ & \ddots & & & & \\ & & 1 & & & \\ & & & \Delta\theta & & \\ & & & & 1 & \\ & & & & & \ddots \; 1 \end{pmatrix} \begin{pmatrix} 1 & & & & & \\ & \ddots & & & & \\ & & 1 & & & \\ & & & \Delta\varphi & & \\ & & & & 1 & \\ & & & & & \ddots \; 1 \end{pmatrix}, \quad (3)$$

where the factors of this product represent by definition the elementary (intrinsic) PSOs of $\mathbb{E}^n$.

As a consequence there exists only two types of elementary PSO* in $\mathbb{E}^n$:

the rotation (PSO^+) through the angle θ, $(\theta \neq \pi)$ in a plane $\mathbb{E}^2$ included in $\mathbb{E}^n$;

the *homothetie* −1 in $\mathbb{E}^r$, subspace of $\mathbb{E}^n$, called 'partial *homothetie* −1' of dimension r in $\mathbb{E}^n$ with the following particular types:

$r=0$ identity of $\mathbb{E}^n$ (PSO^+);

$r=1$ reflection about a hyperplane $\mathbb{E}^{n-1}$ (PSO^-);

$r=2$ rotation through the angle π in $\mathbb{E}^2$ (PSO^+);

$r=n$ (full) *homothetie* −1 in $\mathbb{E}^n$. If n is even, this *homothetie* is a PSO^+ and if n is odd it is a PSO^-.

Geometrical support of the elementary PSOs of $\mathbb{E}^n$

The geometrical support of an elementary PSO of $\mathbb{E}^n$ is, by definition, the subspace of $\mathbb{E}^n$ point-by-point unchanged by this PSO (hence it is the eigensubspace associated with +1 eigenvalue).

For instance, the rotation supports (PSO^+) given as examples in the preceding paragraph are: point 0, axis x, plane xy, space xyz.

As for the partial n-dimensional *homotheties* −1 of $\mathbb{E}^n$, their support is the subspace $\mathbb{E}^{n-r}$ such that $\mathbb{E}^{n-r}$ is the supplementary, thus orthogonal, subspace of $\mathbb{E}^r$. The following examples can be emphasized:

$\mathbb{E}^n$ space for identity;

$\mathbb{E}^{n-1}$ hyperplane for the reflection;

$\mathbb{E}^{n-2}$ subspace, supplementary of (orthogonal to) $\mathbb{E}^2_\pi$ for π rotation;

point 0 for −1 total (n-dimensional) *homothetie.*

Notation of the elementary PSOs of $\mathbb{E}^n$

Elementary PSOs are denoted by means of only one symbol.

Considering elementary rotations, with $\theta \neq \pi$, it is obvious that the choice of a basis implies an orientation of the plane $\mathbb{E}^2_\theta$. We then generalize the Schoenflies notation system but with Hermann–Mauguin symbols. If $\theta = 2\pi/3$ we shall denote the rotations shown in the preceding example by: $3^1_{xy}, 3^1_{yz}, 3^1_{zt}, 3^1_{tu}$. If $\theta = 4\pi/3$ we shall denote them by: $3^2_{xy}, 3^2_{yz}, \ldots$.

* The '*homothetie k*' is the mapping which associates the vector $\mathbf{u}$ with the vector $\mathbf{u}'$ such that $\mathbf{u}' = k\mathbf{u}$.

* A θ rotation in $\mathbb{E}^2_\theta$ may be decomposed into a non-unique and non-commutative product of two reflections onto two hyperplanes. The axes orthogonal to these hyperplanes belong to $\mathbb{E}^2_\theta$ and $\theta/2$ is the angle between them. In the same manner the r-dimensional partial *homothetie* −1 of $\mathbb{E}^n$ can be decomposed into r reflections onto r hyperplanes but this decomposition is, like the previous one, arbitrary and has no geometrical meaning. Furthermore, the eigenvalues characterizing in an intrinsic manner the PSO(2) are +1 (multiplicity q), −1 (multiplicity r), $e^{i\theta}, e^{-i\theta}, e^{i\varphi}, e^{-i\varphi}, \ldots$. For these three reasons, we shall not consider that the reflection about a hyperplane is the unique (super) elementary PSO of $\mathbb{E}^n$ as do Kuntsevich & Belov (1968).

For the r-dimensional *homothetie* -1 of $\mathbb{E}^n$ we denote by: 1^1 the identity ($r=0$); $M^1_{x_{q+1}}$ the reflection* about the hyperplane orthogonal to x_{q+1}($r=1$); $2^1_{x_{q+1}x_{q+2}}$ the rotation π ($r=2$); $\bar{1}^1_{\mathbb{E}_r}$ in general ($2<r<n$); $\bar{1}^1_{\mathbb{E}_n}$ or $\bar{1}^1_n$ as a simplification if $r=n$ and moreover $\bar{1}^1_3$ will be simply written $\bar{1}^1$.

In any case of an elementary PSO notation, the lower index refers to the supplementary (orthogonal) subspace of the PSOs support.

Non-elementary PSOs of $\mathbb{E}^n$

Assume first that $\theta \neq \varphi \neq \psi \neq \ldots \neq k\pi$.

Definition. If the decomposition (3) of one PSO of $\mathbb{E}^n$ admits at least two factors, this PSO is a non-elementary PSO: it is the commutative product of elementary PSOs.

Geometrical support of a non-elementary PSO of $\mathbb{E}^n$

The geometrical support of a non-elementary PSO of $\mathbb{E}^n$ is, by definition, the $(s+1)^{\text{uplet}}$ (or the s^{uplet} if $r=0$) relative to the $(s+1)$ elementary PSOs it is constituted of (see following examples).

Subspaces of $\mathbb{E}^n$ *point-by-point invariant by one non-elementary PSO of* $\mathbb{E}^n$

It is the intersection of the geometrical supports of the elementary PSOs that set up this PSO. (See following concrete examples and see § II for physical applications.)

Notation of non-elementary PSOs of $\mathbb{E}^n$

Several symbols can be used: it is the commutative product of elementary PSOs that sets up this PSO.

Examples of elementary or non-elementary PSOs of $\mathbb{E}^n$

As concrete examples, we give the list of the most general PSOs of $\mathbb{E}^3, \mathbb{E}^4, \mathbb{E}^5$ and we specify their geometrical support, the set of their unchanged points and their notation (we still assume that $\theta \neq \varphi \neq \ldots \neq k\pi$ and $\theta = 2\pi/3$, $\varphi = 2\pi/4$ in order to write these PSOs).

PSOs of $\mathbb{E}^3$

$$\begin{pmatrix} 1 & 0 \\ 0 & \Delta\theta \end{pmatrix}$$

elementary rotation of $\mathbb{E}^3$
support: axis x; notation 3^1_{yz}

$$\begin{pmatrix} \bar{1} & 0 \\ 0 & \Delta\theta \end{pmatrix}$$

general non-elementary PSO$^-$ of $\mathbb{E}^3$
support: plane yz and axis x.

Invariant point: point 0; notation $M^1_x 3^1_{yz} = S^1_3 = \bar{6}^5$.

This is a $2\pi/3$ rotation–reflection that Schoenflies denotes by only one symbol S^1_3. It is equal to the $-2\pi/6$ rotation–reflection that Hermann & Mauguin also denote by only one symbol $\bar{6}^5$.

PSOs of $\mathbb{E}^4$

$$\begin{pmatrix} \Delta\theta & \\ & \Delta\theta \end{pmatrix}$$

general non-elementary rotation of $\mathbb{E}^4$
support: (zt) and (xy)
set of invariant points: point 0
notation $3^1_{xy}4^1_{zt}$

$$\begin{pmatrix} 1 & & \\ & \bar{1} & \\ & & \Delta\theta \end{pmatrix}$$

general non-elementary PSO$^-$ of $\mathbb{E}^4$
support: (xzt) and (xy)
set of invariant points: axis x
notation $M^1_y 3^1_{zt}$.

PSOs of $\mathbb{E}^5$

$$\begin{pmatrix} 1 & & \\ & \Delta\theta & \\ & & \Delta\varphi \end{pmatrix}$$

general non-elementary rotation of $\mathbb{E}^5$
support: (xtu) (xyz)
set of invariant points: axis x
notation $3^1_{yz}4^1_{tu}$

$$\begin{pmatrix} \bar{1} & & \\ & \Delta\theta & \\ & & \Delta\varphi \end{pmatrix}$$

general non-elementary PSO$^-$ of $\mathbb{E}^5$
support: ($yztu$) (xtu) and (xyz)
set of invariant points: point 0
notation: $M^1_x 3^1_{yz} 4^1_{tu}$.

Degenerate and non-degenerate PSOs of $\mathbb{E}^n$

Definition. A PSO is degenerate if at least one of its eigenvalues is a multiple-order root of the characteristic polynomial. It is non-degenerate in the

* M generalizes m of $\mathbb{E}^3$ and recalls that the hyperplane is the mirror upon which the reflection applies.

opposite case (*i.e.* if $q=0$ or 1, $r=0$ or 1, $\theta \neq \varphi \neq \ldots \neq k\pi$).

Thus the general PSOs $\mathbb{E}^3$, $\mathbb{E}^4$, $\mathbb{E}^5$ are non-degenerate when the elementary rotations of $\mathbb{E}^4$ and $\mathbb{E}^5$ are degenerate (eigenvalue 1, with multiplicity 2 and 3, respectively).

The partial *homotheties* -1 of $\mathbb{E}^n$ are always degenerate if $n>2$ [eigenvalues -1 and (or) $+1$ of multiple order].

The identity and the total *homothetie* -1 of $\mathbb{E}^n$ are completely degenerate if $n>1$ (one n-order eigenvalue $+1$ or -1) and their product by another PSO of $\mathbb{E}^n$ is always commutative.

Multiple eigenvalue +1 or −1

In this case, the decomposition (1) is unique and the geometrical support is uniquely defined.

$$\begin{pmatrix} \bar{1}_3 & \\ & \Delta\theta \end{pmatrix}$$

For example: PSO$^-$ of $\mathbb{E}^5$ denoted by $\bar{1}^1_{xyz}3^1_{tu}$ ($\theta = 2\pi/3$).

The support is (tu) and (xyz); the set of invariant points reduces to point 0.

Multiple eigenvalue $e^{i\theta}$ or $e^{i\varphi}, \ldots$

When $n \geq 4$, we may have the following cases, apart from the cases mentioned above:

$$\theta = \varphi \neq \psi \neq \ldots \quad \text{or } \theta = \varphi \neq \psi = \chi \neq \ldots \quad \text{or } \theta = \varphi = \psi \neq \chi \neq \ldots .$$

Then the decomposition (1) is still unique if it is written differently:

$$\mathbb{E}^n = \mathbb{E}^q \oplus \mathbb{E}^r \oplus \mathbb{E}^4_{\theta\theta} \oplus \mathbb{E}^2_{\psi} \oplus \ldots \quad (1')$$

$$\mathbb{E}^n = \mathbb{E}^q \oplus \mathbb{E}^r \oplus \mathbb{E}^4_{\theta\theta} \oplus \mathbb{E}^4_{\psi\psi} \oplus \ldots \quad (1'')$$

$$\mathbb{E}^n = \mathbb{E}^q \oplus \mathbb{E}^r \oplus \mathbb{E}^6_{\theta\theta\theta} \oplus \mathbb{E}^2_{\chi} \oplus \ldots . \quad (1''')$$

An ambiguity appears in the decomposition into elementary PSOs and in the definition of the geometrical support but only inside vector spaces $\mathbb{E}^4, \mathbb{E}^6, \ldots$.

Consider, for instance, the following simple case taken in $\mathbb{E}^4$ with $q=r=0$ and $\theta = \varphi \neq k\pi$.

$$\Delta\theta\Delta\theta = \begin{pmatrix} \Delta\theta & \\ & \Delta\theta \end{pmatrix} \quad \text{where } \Delta\theta = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}. \quad (4)$$

This is a non-elementary degenerate PSO$^+$ equal to the commutative product of two rotations through the angle θ in the two orthogonal planes (x_1x_2) and (x_3x_4). We can show that these two planes of rotation are not unique but belong to a one-parameter family of pairs of orthogonal planes.

Let

$$\mathbf{X}_1 = \lambda\mathbf{x}_1 - \mu\mathbf{x}_3 \quad \mathbf{X}_3 = \mu\mathbf{x}_1 + \lambda\mathbf{x}_3$$
$$\mathbf{X}_2 = \lambda\mathbf{x}_2 + \mu\mathbf{x}_4 \quad \mathbf{X}_4 = -\mu\mathbf{x}_2 + \lambda\mathbf{x}_4$$

with $\lambda, \mu \in \mathbb{R}$ and $\lambda^2 + \mu^2 = 1$.

Under these conditions it can easily be verified that $(\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3, \mathbf{X}_4)$ is a direct orthonormal basis, that $(\mathbf{x}_1, \mathbf{x}_2)(\mathbf{x}_3, \mathbf{x}_4)$ correspond to $\lambda = 1$, $\mu = 0$ and that the planes (X_1, X_2) and (X_3, X_4) are orthogonal [each vector of (X_1, X_2) is orthogonal to each vector of (X_3, X_4)]. Let V be the matrix which transforms the $(\mathbf{x}_i)$ basis into the $(\mathbf{X}_i)$ basis and let V^{-1} be the inverse matrix:

$$V = \begin{pmatrix} \lambda & 0 & -\mu & 0 \\ 0 & \lambda & 0 & \mu \\ \mu & 0 & \lambda & 0 \\ 0 & -\mu & 0 & \lambda \end{pmatrix}$$

$$V^{-1} = \begin{pmatrix} \lambda & 0 & \mu & 0 \\ 0 & \lambda & 0 & -\mu \\ -\mu & 0 & \lambda & 0 \\ 0 & \mu & 0 & \lambda \end{pmatrix} \quad (\det V = 1).$$

In the $(\mathbf{X}_i)$ basis the isometry $\Delta\theta$ matrix is

$$B = V\Delta\theta\Delta\theta V^{-1} = \begin{pmatrix} \Delta\theta & 0 \\ 0 & \Delta\theta \end{pmatrix}.$$

It keeps the same form as (4). Thus, in any $(\mathbf{X}_1, \ldots, \mathbf{X}_4)$ basis corresponding to any couple λ, μ ($\lambda^2 + \mu^2 = 1$) the PSO matrix is the same reduced orthogonal matrix (4).*

This result can easily be generalized to other cases of degeneration. The 'reduction' bases then differ, not only by the arbitrary choice of pairs of basis vectors chosen in the uniquely defined planes, but also by the arbitrary choice of pairs of orthogonal planes chosen in uniquely defined families in $\mathbb{E}^4_{\theta\theta}, \mathbb{E}^6_{\theta\theta\theta}, \ldots$; only $\mathbb{E}^4_{\theta\theta}, \mathbb{E}^6_{\theta\theta\theta}, \ldots$ spaces are uniquely defined.

Any notation in the form $M^1_{x_2}4^1_{x_3x_4}4^1_{x_5x_6}3^1_{x_7x_8}$ involves an arbitrary choice (the choice of x_i for $3 \leq i \leq 6$).

II. The crystallographic PSO of $\mathbb{E}^n$

Crystallographic PSOs are those PSOs compatible with the perodicity of the crystal lattice in $\mathbb{E}^n$ (Weigel & Berar, 1978).

We shall first detail the crystallographic PSO of $\mathbb{E}^4$. Let Ω be a general PSO$^+$; in a 'reduction' basis it is described by the matrix

$$A = \begin{pmatrix} \cos\theta & -\sin\theta & 0 & 0 \\ \sin\theta & \cos\theta & 0 & 0 \\ 0 & 0 & \cos\varphi & -\sin\varphi \\ 0 & 0 & \sin\varphi & \cos\varphi \end{pmatrix}.$$

* This double rotation through the angle θ in two orthogonal planes is called a 'Clifford displacement' (Coxeter, 1973).

Table 1. *The five geometrical symbols of the crystallographic PSOs of* $\mathbb{E}^2$, $\mathbb{E}^3$, $\mathbb{E}^4$

	$PSO^+\mathbb{E}^2$		$PSO^+\mathbb{E}^3$	$PSO^-\mathbb{E}^3$		$PSO^-\mathbb{E}^4$	Hurley	Hermann
degenerate	1		1	M_z^1	*	M_t^1	T	2 1 1 1
	2_{xy}^1	*	2_{yz}^1	$\bar{1}^1$	*	$\bar{1}_{yzt}^{-1}$	T'	2 2 2 1
non-degenerate	$4_{xy}^{\pm 1}$	*	$4_{yz}^{\pm 1}$	$M_x^1 4_{yz}^{\pm 1}$		$M_y^1 4_{zt}^{\pm 1}$	F	4 2 1
	$6_{xy}^{\pm 1}$	*	$6_{yz}^{\pm 1}$	$M_x^1 6_{yz}^{\pm 1}$		$M_y^1 6_{zt}^{\pm 1}$	N	6 2 1
	$3_{xy}^{\pm 1}$	*	$3_{yz}^{\pm 1}$	$M_x^1 3_{yz}^{\pm 1}$		$M_y^1 3_{zt}^{\pm 1}$	N'	3 2 1

Notes:
Hurley and Hermann notations are valid only in $\mathbb{E}^4$.
The elementary PSOs are indicated by an asterisk (*).
The identity 1 is a trivial PSO, for which it is of no interest to detail the elementary or non-elementary characters.
On the contrary, the identity 1 and the total *homothetie* -1 are fully degenerate PSOs.

Its characteristic polynomial is

$$\det(A-\lambda I)=\lambda^4-2(\cos\varphi+\cos\theta)\lambda^3 +2(1+2\cos\varphi\cos\theta)\lambda^2 -2(\cos\varphi+\cos\theta)\lambda+1.$$

Now considering a basis erected with the definition vectors of a primitive cell of a crystal lattice, it appears that the characteristic polynomial Ω has only integral positive or negative coefficients.

It can be seen that if (θ, φ) is a solution, so is (φ, θ) and $(\pi-\theta, \pi-\varphi)$. Thus it is sufficient to look for a relation satisfying $\cos\varphi+\cos\theta\geq 0$.

Let

$$2(\cos\varphi+\cos\theta)=k,\ k\in\mathbb{N}$$
$$2(1+2\cos\varphi\cos\theta)=k',\ k'\in\mathbb{Z}.$$

Then $\cos\varphi$ and $\cos\theta$ are solutions of the equation

$$X^2-\frac{k}{2}X+\frac{1}{2}\left(\frac{k'}{2}-1\right)=0,$$

where X' and X'' roots must belong to $[-1, 1]$.

A simple reasoning gives as possible values for k and k' the following:

k	0	1	2	3	4
k'	$-2, -1, 0, 2$	$0, 1, 2$	$2, 3$	4	6

Since the general PSO^- of $\mathbb{E}^4$ in a 'reduction' basis is described by

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & 0 \\ 0 & 0 & \cos\theta & -\sin\theta \\ 0 & 0 & \sin\theta & \cos\theta \end{pmatrix},$$

then it can rapidly be verified that the various types of PSO^- of $\mathbb{E}^4$ are strictly similar to the five types of PSO^- of $\mathbb{E}^3$ (see Table 1).

In the same way it can be shown that the various types of PSO^+ of $\mathbb{E}^5$ and PSO^- of $\mathbb{E}^5$ and of $\mathbb{E}^6$ are strictly similar to the 19 types of PSO^+ of $\mathbb{E}^4$ (Table 2).

In fact, a 'reduction' basis, the PSOs of $\mathbb{E}^5$ and $\mathbb{E}^6$ are described by

$$\left(\begin{array}{c|cccc} \bar{1} & 0 & 0 & 0 & 0 \\ \hline 0 & & & & \\ 0 & & & & \\ 0 & & A & & \\ 0 & & & & \end{array}\right)$$

$$\left(\begin{array}{cc|cccc} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & & & & \\ 0 & 0 & & A & & \\ 0 & 0 & & & & \\ 0 & 0 & & & & \end{array}\right),$$

where A denotes the matrix of the PSO^+ of $\mathbb{E}^4$ written above.

The numbers of different types of PSO in n-dimensional spaces are given in Table 3.

Conclusion

The description of the PSOs of $\mathbb{E}^4$ and of their geometric support is useful in physics in particular for the counting of polar groups. In fact all PSO elements of such a group must leave at least one vector of the space $\mathbb{E}^n$ unchanged: the electric polarization vector. If the invariant point-by-point subspace of only one PSO of a crystallographic group is reduced to a point, this group cannot be polar: such a PSO is called 'non-polar'. Thus

3_{xy}^1 is non-polar in $\mathbb{E}^2$
$6_{yz}^1=M_x^1 3_{yz}^1$ is non-polar in $\mathbb{E}^3$
$8_{\alpha\beta}^1 8_{\gamma\delta}^1$ is non-polar in $\mathbb{E}^4$, and so on.

Through these geometric points of view, we have proved there are 32 point crystallographic polar groups in $\mathbb{E}^4$ and 227 in $\mathbb{E}^5$ (Weigel & Veysseyre, 1982); we expound these results in connection with the point

Table 2. *The nineteen geometrical symbols of the crystallographic PSO of* $\mathbb{E}^4$, $\mathbb{E}^5$, $\mathbb{E}^6$

	Hurley	Hermann	PSO$^+\mathbb{E}^4$		PSO$^+\mathbb{E}^5$	PSO$^-\mathbb{E}^5$		PSO$^-\mathbb{E}^6$
degenerate	D	44	$4^{\pm1}_{xy}4^{\pm1}_{zt}$		$4^{\pm1}_{yz}4^{\pm1}_{tu}$	$M^1_x4^{\pm1}_{yz}4^{\pm1}_{tu}$		$M^1_y4^{\pm1}_{zt}4^{\pm1}_{uv}$
	S	33	$3^{\pm1}_{xy}3^{\pm1}_{zt}$		$3^{\pm1}_{yz}3^{\pm1}_{tu}$	$M^1_x3^{\pm1}_{yz}3^{\pm1}_{tu}$		$M^1_y3^{\pm1}_{zt}3^{\pm1}_{uv}$
	S'	66	$6^{\pm1}_{xy}6^{\pm1}_{zt}$		$6^{\pm1}_{yz}6^{\pm1}_{tu}$	$M^1_x6^{\pm1}_{yz}6^{\pm1}_{tu}$		$M^1_y6^{\pm1}_{zt}6^{\pm1}_{uv}$
	I	1111	1		1	M^1_u	*	M^1_v
	I'	2222	$\bar{1}^1_4$	*	$\bar{1}^1_{yztu}$	$\bar{1}^1_5$	*	$\bar{1}^1_{yztuv}$
non-degenerate	K	311	$3^{\pm1}_{zt}$	*	$3^{\pm1}_{tu}$	$M^1_z3^{\pm1}_{tu}$		$M^1_t3^{\pm1}_{uv}$
	E	2211	$2^{\pm1}_{zt}$	*	$2^{\pm1}_{tu}$	$M^1_z2^{\pm1}_{tu}$		$M^1_t2^{\pm1}_{uv}$
	R	411	$4^{\pm1}_{zt}$	*	$4^{\pm1}_{tu}$	$M^1_z4^{\pm1}_{tu}$		$M^1_t4^{\pm1}_{uv}$
	Z	611	$6^{\pm1}_{zt}$	*	$6^{\pm1}_{tu}$	$M^1_z6^{\pm1}_{tu}$		$M^1_t6^{\pm1}_{uv}$
	A	8	$8^{\pm1}_{xy}8^{\pm3}_{zt}$		$8^{\pm1}_{yz}8^{\pm3}_{tu}$	$M^1_x8^{\pm1}_{yz}8^{\pm3}_{tu}$		$M^1_y8^{\pm1}_{zt}8^{\pm3}_{uv}$
	B	63	$6^{\pm1}_{xy}3^{\pm1}_{zt}$		$6^{\pm1}_{yz}3^{\pm1}_{tu}$	$M^1_x6^{\pm1}_{yz}3^{\pm1}_{tu}$		$M^1_y6^{\pm1}_{zt}3^{\pm1}_{uv}$
	C	T	$12^{\pm1}_{xy}12^{\pm5}_{zt}$		$12^{\pm1}_{yz}12^{\pm5}_{tu}$	$M^1_x12^{\pm1}_{yz}12^{\pm5}_{tu}$		$M^1_y12^{\pm1}_{zt}12^{\pm5}_{uv}$
	K'	622	$6^{\pm1}_{xy}2^{\pm1}_{zt}$		$6^{\pm1}_{yz}2^{\pm1}_{tu}$	$M^1_x6^{\pm1}_{yz}2^{\pm1}_{tu}$		$M^1_y6^{\pm1}_{zt}2^{\pm1}_{uv}$
	L	10	$10^{\pm1}_{xy}10^{\pm3}_{zt}$		$10^{\pm1}_{yz}10^{\pm3}_{tu}$	$M^1_x10^{\pm1}_{yz}10^{\pm3}_{tu}$		$M^1_y10^{\pm1}_{zt}10^{\pm3}_{uv}$
	L'	5	$5^{\pm1}_{xy}5^{\pm2}_{zt}$		$5^{\pm1}_{yz}5^{\pm2}_{tu}$	$M^1_x5^{\pm1}_{yz}5^{\pm2}_{tu}$		$M^1_y5^{\pm1}_{zt}5^{\pm2}_{uv}$
	M	64	$6^{\pm1}_{xy}4^{\pm1}_{zt}$		$6^{\pm1}_{yz}4^{\pm1}_{tu}$	$M^1_x6^{\pm1}_{yz}4^{\pm1}_{tu}$		$M^1_y6^{\pm1}_{zt}4^{\pm1}_{uv}$
	M'	43	$4^{\pm1}_{xy}3^{\pm1}_{zt}$		$4^{\pm1}_{yz}3^{\pm1}_{tu}$	$M^1_x4^{\pm1}_{yz}3^{\pm1}_{tu}$		$M^1_y4^{\pm1}_{zt}3^{\pm1}_{uv}$
	R'	422	$4^{\pm1}_{xy}2^{\pm1}_{zt}$		$4^{\pm1}_{yz}2^{\pm1}_{tu}$	$M^1_x4^{\pm1}_{yz}2^{\pm1}_{tu}$		$M^1_y4^{\pm1}_{zt}2^{\pm1}_{uv}$
	Z'	322	$3^{\pm1}_{xy}2^{\pm1}_{zt}$		$3^{\pm1}_{yz}2^{\pm1}_{tu}$	$M^1_x3^{\pm1}_{yz}2^{\pm1}_{tu}$		$M^1_y3^{\pm1}_{zt}2^{\pm1}_{uv}$

Notes: As for Table 1.

Table 3. *Number of different types of PSO in n-dimensional spaces with* $n \le 10$

Dimension of $\mathbb{E}^n$	0	1	2	3	4	5	6	7	8	9	10
PSO$^+$	1	1	5	5	19	19	59	59	165	165	
PSO$^-$		1	1	5	5	19	19	59	59	165	165

groups of incommensurate phases in $\mathbb{E}^4$, $\mathbb{E}^5$, $\mathbb{E}^6$ in the next paper of this series (Veysseyre, Weigel, Phan & Effantin, 1984).

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APPENDIX

Let $\mathbf{E}$ be an n-dimensional vector space over $\mathbb{C}$, $\mathbb{E}$ be the corresponding affine space, φ an orthogonal mapping of $\mathbf{E}$ associated with a point isometry of $\mathbb{E}$ and I the identity mapping of $\mathbf{E}$.

$\mathbf{X}$, a non-zero vector of $\mathbf{E}$, is an eigenvector of φ if there exists a complex number λ such that $\varphi(\mathbf{X}) = \lambda\mathbf{X}$; λ is called the eigenvalue associated with $\mathbf{X}$.

The characteristic polynomial of φ is the polynomial $\det(\varphi - \lambda I)$.

Let $B = (\mathbf{e}_1, \ldots, \mathbf{e}_n)$ be a basis of $\mathbf{E}$ and $\Phi = (a_{ij})_{ij}$, the matrix of φ, in this basis, is

$$\Phi = \begin{pmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & & \vdots \\ a_{n1} & \cdots & a_{nn} \end{pmatrix}.$$

The columns consist of the vectors $\varphi(\mathbf{e}_i)$ in the basis B:

$$\det(\varphi - \lambda I) = \begin{vmatrix} a_{11} - \lambda & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} - \lambda & \cdots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} - \lambda \end{vmatrix}.$$

The characteristic polynomial expression is independent of the basis B chosen in $\mathbf{E}$; λ is the eigenvalue of φ if and only if it is a root of the characteristic polynomial of φ. Then φ admits n complex eigenvalues distinct or non-distinct, the eigenvalue product is $\det \varphi$, their sum is trace $\varphi = \sum_{i=1}^{n} a_{ii}$.

The eigensubspace associated with the eigenvalue λ is composed of the null vector $\mathbf{0}$ and of the eigenvectors associated with λ.

The eigensubspace associated with the eigenvalue 1 is the set of invariant vectors of φ.

Theorem

There exists an orthonormal basis of $\mathbf{E}$ in which the matrix of φ is

$$\begin{pmatrix} I_q & & & & \\ & \bar{I}_r & & & \\ & & \Delta\theta_1 & & \\ & & & \ddots & \\ & & & & \Delta\theta_n \end{pmatrix}$$

I_q: identity q-dimensional matrix; $\bar{I}_r$: *homothetie* -1 r-dimensional matrix;

$$\Delta\theta_k = \begin{pmatrix} \cos\theta_k & -\sin\theta_k \\ \sin\theta_k & \cos\theta_k \end{pmatrix};$$

$q+r+2s=n$.

Let $B=(\mathbf{e}_1,\ldots,\mathbf{e}_n)$ be an orthonormal basis of $\mathbb{E}$.

By means of B, $\mathbb{E}^n$ can be identified with $\mathbb{R}^n$. By means of canonical injective mapping: $\mathbb{R}\to\mathbb{C}$, $\mathbb{R}^n$ can be identified with a subspace of $\mathbb{C}^n$.

The restriction to $\mathbb{R}^n\times\mathbb{R}^n$ of the Hermitian scalar product of $\mathbb{C}^n$ is the Euclidean scalar product of $\mathbb{E}$.

In the basis B the matrix of φ is orthogonal and real: ${}^tAA=I$. Over $\mathbb{C}^n$ it defines a unitary operator Φ. Real eigenvalues of Φ are 1 and -1, non-real eigenvalues are 2 by 2 conjugate: they all have a modulus of 1. Let us settle then with the following sequence:

$$1,1,\ldots,1,-1,\ldots,-1,e^{i\theta_1},\ldots,e^{i\theta_s},e^{-i\theta_s}.$$

Since Φ is unitary, there exists an orthonormal basis of eigenvectors of Φ. Eigensubspaces associated with two non-real eigenvalues are orthogonal. We can choose eigenvectors 2 by 2 conjugate, making up a basis of these subspaces. Real vectors can be chosen as eigenvectors corresponding to eigenvalues 1 and -1. Hence we have an orthonormal basis of $\mathbb{C}^n$:

$$g_1,\ldots,g_{q+r},f_1,\bar{f}_1,\ldots,f_k,\bar{f}_k,\ldots,f_s,\bar{f}_s.$$

We write:

$$\left.\begin{aligned} g_{q+r+2k-1} &= \frac{1}{\sqrt{2}}(f_k+\bar{f}_k) \\ g_{q+r+2k} &= \frac{i}{\sqrt{2}}(f_k-\bar{f}_k) \end{aligned}\right\} \quad 1\le k\le s.$$

Then $(g_1,\ldots,g_n)$ is a real orthonormal basis of $\mathbb{C}^n$ and an orthonormal basis of $\mathbb{R}^n$.

In this basis the matrix of Φ is the matrix of φ and it is written as given in the theorem.

$$\begin{aligned} \varphi(g_{q+r+2k-1}) &= \frac{1}{\sqrt{2}}[\varphi(f_k)+\varphi(\bar{f}_k)] \\ &= \frac{1}{\sqrt{2}}[e^{i\theta_k}f_k+e^{-i\theta_k}\bar{f}_k] \\ &= \cos\theta\, g_{q+r+2k-1} \\ &\quad + i\sin\theta\left(\frac{1}{\sqrt{2}}f_k-\frac{1}{\sqrt{2}}\bar{f}_k\right) \\ &= \cos\theta\, g_{q+r+2k-1} + i\sin\theta\, g_{q+r+2k}. \end{aligned}$$

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