Concept of a multimetrical space group

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A multimetrical space group G is the symmetry group of a pattern having lattice periodicity in an affine space made multimetrical by attaching to it a set of metrics of different signature. The Euclidean metric tensor is always supposed to be a member of the set. The point group K of G is generated by elements leaving the lattice invariant and transforming some of the metric tensors of the set into another one of the same set. When the pattern describes a crystal structure in the point-atom approximation, the Euclidean subgroup G_0 of G is the space group of the crystal. When the pattern is defined in superspace, i.e., is obtained by the embedding of a quasicrystal structure (as in the cut-projection method), the subgroup G_{SR} of G leaving the (lower-dimensional) physical space invariant is the scale-space group of the quasicrystal.

I. INTRODUCTION

The search for an appropriate characterization of the possible symmetries of quasicrystals in terms of crystallographic groups leads to considering the embedding of the structure in a higher-dimensional Euclidean space (the superspace) according to the rule

$$\rho(r) \overset{\mathrm{FT}_3}{\longleftrightarrow} \hat{\rho}(h_1, \ldots, h_n) \equiv \hat{\rho}_s(h_1, \ldots, h_n) \overset{\mathrm{FT}_n}{\longleftrightarrow} \rho_s(r_s) \qquad (1)$$

where FT_n denotes the n-dimensional Fourier transform.[1–5]

In that way the $\mathbb{Z}$-module properties of the diffraction pattern and the rotational symmetries, together with associated extinctions rules due to corresponding nonprimitive translations, are properly taken into account by means of a higher dimensional space group (the superspace group). One misses, however, scaling symmetries like those found in tiling models obeying so-called inflation and deflation rules typical for a one-dimensional Fibonacci sequence, or for a two-dimensional Penrose tiling.[6]

Actually, the same superspace approach also allows the description of these transformations in terms of invertible matrices with integral entries mapping injectively the embedded structure into itself. It is even possible, by adopting a direct space embedding in the superspace which essentially corresponds to the so-called cut-projection method,[7,8] to describe the quasicrystal in terms of a higher-dimensional structure which is invariant with respect to those transformations.[9–11] It is then justified to speak of crystallographic point-group symmetries which induce in the quasicrystal structure scaling transformations.

Looking for a crystallographic group allowing to take into account both the rotational and the scaling symmetries, one then arrives at the scale-space group, which contains as a Euclidean subgroup the superspace group of the embedded structure.[12,13]

The author believes that beside lattice translational symmetry, metrical invariance is an essential ingredient of a crystallographic symmetry group. From this point of view, there is a serious problem, because the scaling transformations considered above do leave a (higher-dimensional) lattice invariant but, being of infinite order, are incompatible with a Euclidean metric g_e in superspace.

Exploring the well-known models for the observed quasicrystal structures (in one, two and three dimensions) one sees how an indefinite metric tensor g_i can be attached to a basis of the lattice of the embedded structures, in such a way that the scaling integral matrices leave that metric tensor invariant (possibly up to a sign).[14] Scaling invariance is then associated to automorphs (or to negautomorphs) of an indefinite integral quadratic form.[15–17]

Two ways are then open for not giving up these metrical invariances, i.e., that for the scaling and that for the rotational symmetries. (i) Following the first way, one simply increases the number of dimensions of the superspace: In particular, a space of $2n$-dimensions with a metric tensor $g_e \oplus g_i$ will do the job. (ii) In the second way, the superspace dimension considered is a minimal one (equal thus to the rank n of the $\mathbb{Z}$-module), and one attaches more than one metric tensor to the same superspace that was at first considered an affine space in which the lattice translational symmetries are well defined.

Here, the second approach will be followed and this eventually leads to the concept of multimetrical space group. One can then forget the quasicrystals, the superspace and all that, and simply consider periodic patterns of given dimension admitting a multimetrical space group as symmetry. One then recognizes the potential applicability of this concept to normal (i.e., commensurate) three-dimensional crystals.

For a precise definition of the mathematical concepts underlying n-dimensional crystallography and used here without a particular explanation, the reader is referred to the book by W. Opechowski on crystallographic and metacrystallographic groups.[18]

II. MULTIMETRICAL SPACE

Consider an n-dimensional affine space V and a basis $\{e_1,\ldots,e_n\}$ orthonormal with respect to a set of metric tensors $\{g_\nu^0\}$ with $\nu=1,\ldots,2^n$:

$$e_i \overset{\nu}{\circ} e_j = (g_\nu^0)_{ij} = \epsilon_{\nu ij} = \pm\delta_{ij} \ , \tag{2}$$

where the different scalar products are denoted by $\overset{\nu}{\circ}$, respectively. Accordingly, the g_ν^0 tensors are diagonal with ± 1 as diagonal elements and will be called admissible metric tensors. The corresponding orthogonal groups are denoted by $O_\nu(n)$ and the inhomogeneous ones by $IO_\nu(n)$.

By convention, the $\nu=0$ case will be used for the Euclidean metric, and in that case the scalar product symbol is generally simply omitted. It is worth noting the simple matrix relation:

$$(g_\nu^0)^2 = g_0^0 \ . \tag{3}$$

A. Multimetrical lattices

Consider in V a lattice Λ with basis $a_1,\ldots,a_n$:

$$a_i = \sum_{j=1}^{n} e_j \alpha_{ji} \tag{4}$$

having attached a set of metric tensors $g(\Lambda)=\{g_\nu\}$.

$$(g_\nu)_{ij} = a_i \overset{\nu}{\circ} a_j \ . \tag{5}$$

In matrix notation and denoting transposition by a "tilde" one simply has

$$g_\nu = \tilde{\alpha} g_\nu^0 \alpha \ . \tag{6}$$

In particular for $n=2$, one gets a corresponding binary quadratic form (a,b,c):

$$g_\nu = (a,b,c) = \begin{bmatrix} a & \frac{b}{2} \\ \frac{b}{2} & c \end{bmatrix} . \tag{7}$$

Then this set of metric tensors is said to be a compatible set with respect to Λ. Let us remark that in many cases, while considering the multimetrical symmetry of a periodic pattern (a concept made more precise below) it is not necessary to consider a complete set of compatible metric tensors, a subset of these very often suffices. In what follows, we will assume that such a subset always includes the Euclidean metric tensor g_0.

B. Multimetrical transformations

For a given set of compatible metric tensors $g(\Lambda)$ of a lattice Λ, admitted multimetrical transformations A have to satisfy the set of coupled conditions:

$$\tilde{A} g_\nu A = g_\mu, \quad \tilde{A} g_\mu A = g_\nu \tag{8}$$

for some $g_\nu, g_\mu \in g(\Lambda)$ and $A \in Gl(n,\mathbb{Z})$.

This definition deserves a comment. Quite naturally, one is led to consider only transformations leaving one metric tensor of the set invariant. Say,

$$\tilde{A} g_\mu A = g_\mu \ . \tag{9}$$

As one knows from the theory of integral binary quadratic forms already, that is not enough for a proper characterization of the invariant transformations. If g_μ is indefinite there are cases where negautomorphs play an important role. They are in fact negative units of a corresponding quadratic field.[19–21] For a negautomorph A of g_μ one has

$$\tilde{A} g_\mu A = -g_\mu \ . \tag{10}$$

For dimensions higher than two, direct sum operation has also to be admitted. Suppose now that one has $g_\rho = g_\mu \oplus \mathbb{1}$, then $B = A \oplus \mathbb{1}$ is neither an automorph, nor a negautomorph of g_ρ and it requires a transformation law like

$$\tilde{B} g_\rho B = g_\nu, \quad \text{with } g_\nu = -g_\mu \oplus \mathbb{1} \ . \tag{11}$$

In this case, the two relations of Eq. (8) are satisfied. In general, Eq. (8) expresses the condition that the admitted multimetrical transformations correspond to a direct sum of automorphs and/or negautomorphs of the compatible metrical tensors (including the lower dimensional ones).

The holohedry H of Λ for given $g(\Lambda)$ is then the subgroup of $Gl(n,\mathbb{Z})$ generated by all $g(\Lambda)$-multimetrical transformations. The product of two multimetrical transformations need not to be multimetrical, but if two multimetrical transformations leave a pattern invariant, so does their product.

Before proceeding further and introducing concepts like multimetrical point and space groups, it is appropriate to give a concrete example in order to help achieve a better understanding of the present approach.

C. A first example of multimetrical transformations

Considered is a two-dimensional affine space V with basis vectors e_1, e_2. The admitted metric tensors are

$$g_0^0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad g_1^0 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad g_2^0 = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}, \quad g_3^0 = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} . \tag{12}$$

A lattice Λ with basis vectors a_1, a_2 is defined

$$\begin{aligned} a_1 &= \alpha_{11} e_1 + \alpha_{21} e_2 = (\alpha_{11}, \alpha_{21}) \ , \\ a_2 &= \alpha_{12} e_1 + \alpha_{22} e_2 = (\alpha_{12}, \alpha_{22}) \ . \end{aligned} \tag{13}$$

Parametrizing the entries of the matrix α as

$$\alpha = \begin{bmatrix} \cosh\chi & -\sinh\chi \\ \sinh\chi & \cosh\chi \end{bmatrix} \text{ with } \tanh\chi = \sqrt{5} - 2 \ , \tag{14}$$

one gets a Λ-compatible metric set $g(\Lambda) = \{g_0, g_1, g_2\}$ where

$$g_0=\tilde{\alpha}g_0^0\alpha=\frac{\sqrt{5}}{2}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix},$$

$$g_1=\tilde{\alpha}g_1^0\alpha=\begin{bmatrix}1 & -\frac{1}{2}\\ -\frac{1}{2} & -1\end{bmatrix}, \tag{15}$$

$$g_2=-g_1 .$$

We now consider the following multimetrical transformations:

$$A=\begin{bmatrix}-1 & 0\\ 0 & 1\end{bmatrix},\quad B=\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix},$$

$$C=\begin{bmatrix}1 & 0\\ -1 & -1\end{bmatrix},\quad D=\begin{bmatrix}1 & -1\\ 0 & -1\end{bmatrix}. \tag{16}$$

The corresponding invariance of the various metric tensors is given by

$$\tilde{A}g_0A=g_0,\quad \tilde{B}g_0B=g_0, \tilde{C}g_1C=g_1,\quad \tilde{D}g_1D=g_1 , \tag{17}$$

so that the multimetrical condition Eq. (8) is satisfied. These are all improper automorphs of the quadratic forms involved.

The subgroup K of $Gl(2,\mathbb{Z})$ given in terms of the set of generators

$$K=\{A,B,C,D\} \tag{18}$$

is then a multimetrical point group of the lattice Λ.

These generators are not the only multimetrical point group transformations. Indeed, an additional improper negautomorph, which is in fact the Fibonacci transformation matrix, can be expressed as product $F=ABC$, the square of which $F^2=DC$ is an hyperbolic rotation by $\phi=2\ln\tau$ with $\tau=(1+\sqrt{5})/2$ the golden number. Furthermore, the Euclidean rotation by $\pi/2$ is expressible as $E=AB$ and appears to be at the same time an automorph of the Euclidean binary form (1,0,1) and a negautomorph of the indefinite quadratic form $(1,-1,-1)$. We thus have with

$$F=\begin{bmatrix}1 & 1\\ 1 & 0\end{bmatrix},\quad E=\begin{bmatrix}0 & -1\\ 1 & 0\end{bmatrix} \tag{19}$$

the corresponding metrical relations:

$$\tilde{E}g_0E=g_0,\quad \tilde{E}g_1E=g_2,\quad \tilde{E}g_2E=g_1 ,$$

$$\tilde{F}g_1F=g_2,\quad \tilde{F}g_2F=g_1 , \tag{20}$$

which all are admitted multimetrical transformations of the lattice Λ.

III. MULTIMETRICAL SPACE GROUPS

A multimetrical space group G in n dimensions is a subgroup of the affine group $A(n)$ defined in terms of the following: an n-dimensional lattice translation subgroup Λ; a point group K, subgroup of the holohedry H of Λ with respect to a set $g(\Lambda)$ of compatible metric tensors; a system of nonprimitive translations $v(K)$ satisfying the Frobenius congruence relations

$$v(AB)\equiv v(A)+Av(B)(\mathrm{mod}\Lambda)\quad (\text{for } A,B\in K) \tag{21}$$

for a normalized v: $v(\mathbb{1}_n)=0$. In this definition no distinction is made between the two different concepts of lattice and of lattice group translations.

A general element of the multimetrical space group $G=\{\Lambda,g(\Lambda),K,v(K)\}$ can be written (in the Seitz notation) as

$$g=\{A|a+v(a)\} \tag{22}$$

with $A\in K, a\in\Lambda$, and $v(a)\in v(K)$, the product rule being that of the elements of $A(n)$:

$$gg'=\{AA'|a+v(A)+A[a'+v(A')]\} . \tag{23}$$

In the same way as for space groups, the only translations are lattice translations spanning the n-dimensional space V

$$\{\mathbb{1}_n|a+v(\mathbb{1}_n)\}=a\in\Lambda . \tag{24}$$

The group of lattice translations is, therefore, normal in G. The factor group G/Λ is isomorphic to K, so that G is a group extension of Λ by K. Inequivalent group extensions can be obtained from the elements of the second cohomology group $H_2(K,\mathbb{Z}^n)$.[22]

Change in the choice of the origin of the space V transforms a system of nonprimitive translations into an equivalent one:

$$v'(A)=v(A)+(A-\mathbb{1}_n)f\quad (\text{for } f\in V) . \tag{25}$$

Furthermore, as such systems obey the Frobenius congruence relation (21) and are defined only as modulo lattice translations, inequivalent systems of nonprimitive translations appear as elements of the first cohomology group $H_1(K,\mathbb{R}^n/\mathbb{Z}^n)$, the unit element of which yields the semidirect product of Λ by K.[23] The general situation is, however, very much different from the corresponding one for space groups, where these two cohomology groups are isomorphic. Here, the point group K is not finite. (This is the normal situation, the special case of K finite not being considered here, because it is fairly trivial from a multimetrical point of view.) Therefore the two cohomology groups are, in general, not isomorphic:

$$H_1(K,\mathbb{R}^n/\mathbb{Z}^n)\not\simeq H_2(K,\mathbb{Z}^n) . \tag{26}$$

These two groups are, however, related by a connecting homorphism appearing in a long exact sequence of cohomology groups.[23]

IV. EXAMPLES OF MULTIMETRICAL SPACE GROUPS

A. A first example

A first example reflects the properties of a quasiperiodic chain that one gets from a strip-projection of an hexagonal lattice. The dimension of V is 2 and the set of admitted metric tensors is as in Eq. (12). The lattice Λ is generated by the two basis vectors

$$a_1=(1,0),\quad a_2=\left(\frac{1}{2},\frac{\sqrt{3}}{2}\right) \tag{27}$$

so that one gets the two quadratic forms: the Euclidean one (1,1,1) of the hexagonal lattice, and the indefinite one $(2,2,-1)$ of the lattice denoted as $\overline{M}_4$ within the framework of two-dimensional relativistic crystallography.[16] The corresponding two metric tensors are

$$g_0=\begin{bmatrix}1 & \frac{1}{2}\\ \frac{1}{2} & 1\end{bmatrix},\quad g_1=\begin{bmatrix}1 & \frac{1}{2}\\ \frac{1}{2} & -\frac{1}{2}\end{bmatrix}. \tag{28}$$

The generators of the point group K are

$$A=\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix},\quad B=\begin{bmatrix}1 & 1\\ 0 & -1\end{bmatrix},\quad C=\begin{bmatrix}1 & 0\\ 2 & -1\end{bmatrix}, \tag{29}$$

and we can denote this point group by

$$K=\{A,B,C\}=6m\hat{4}\hat{m}. \tag{30}$$

The symbol $\hat{m}$ is used for indicating a hyperbolic mirror. A pair of such mirrors generates a hyperbolic rotation, in quite the same way as the product of two Euclidean mirrors conventionally denoted by the letter m generate a rotation. Indeed, the group K contains a sixfold rotation by an angle $\phi=\pi/3$.

$$E=AB=\begin{bmatrix}0 & -1\\ 1 & 1\end{bmatrix}=6, \tag{31}$$

and a hyperbolic rotation by $\phi=\ln(2+\sqrt{3})$ having a trace equal to $2\cosh\phi=4$

$$F=CB=\begin{bmatrix}1 & 1\\ 2 & 3\end{bmatrix}=\hat{4}. \tag{32}$$

The Euclidean mirrors are given by the generators A and B and the hyperbolic ones by B and by C. In the present case we thus have:

$$m=A,\quad \hat{m}=C, m'=\hat{m}'=B. \tag{33}$$

The compatibility between the sets of metric tensors $g(\Lambda)$ becomes visible, through the common generator B;

$$\tilde{A}g_0A=g_0,\quad \tilde{B}g_0B=g_0,\quad \tilde{B}g_1B=g_1,\quad \tilde{C}g_1C=g_1. \tag{34}$$

From a semidirect product of Λ by K, one gets then the symmorphic multimetrical space group:

$$G=p6m\hat{4}\hat{m}=\{a_1,a_2,A,B,C\}. \tag{35}$$

In general and for a given metrical tensor g_ν, an n-dimensional mirror is an isometry characterized by an eigenvector with eigenvalue $\lambda_-=-1$ perpendicular (according to g_ν) to an invariant hyperplane of dimension $n-1$ called the mirror plane. It is thus an orthogonal reflection element of the group $O(\nu)$.

In the present case, these reflections are determined by two lines along the eigenvectors having eigenvalue 1 and -1, respectively. For a Euclidean mirror, the two lines intersect at 90°, whereas for a hyperbolic mirror they form equal angles with respect to the light cone.

The point group $6m\hat{4}\hat{m}$ is thus generated by reflections and represents the multimetrical generalization of a Coxeter group.

B. A second example

One gets a second example by looking at a superspace embedding on a square lattice of an octagonal chain, i.e., at the chain defined in terms of vertices of the two-dimensional octagonal tiling aligned along a given direction[24] (see Fig. 1). Again the dimension of V is two and the set of admitted metric tensors is as in Eq. (12). The basis of the given lattice Λ is parametrized as in Eq. (14) but now with the χ value given by

$$\tanh\chi=\sqrt{2}-1.$$

Accordingly, one finds for the Λ-compatible set of metric tensors $g(\Lambda)$

$$g_0=\sqrt{2}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix},\quad g_1=\begin{bmatrix}1 & -1\\ -1 & -1\end{bmatrix},\quad g_2=-g_1. \tag{36}$$

The holohedry of Λ with respect to the Euclidean g_0 is generated by

$$A=\begin{bmatrix}-1 & 0\\ 0 & 1\end{bmatrix},\quad B=\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}, \tag{37}$$

yielding $4mm$. The automorphs of g_1 and of g_2, respectively, are generated by

$$C=\begin{bmatrix}1 & 0\\ -2 & -1\end{bmatrix},\quad D=\begin{bmatrix}1 & -2\\ 0 & -1\end{bmatrix}, \tag{38}$$

which are again hyperbolic mirrors. Indeed

$$CD=\begin{bmatrix}1 & -2\\ -2 & 5\end{bmatrix}=\hat{6} \tag{39}$$

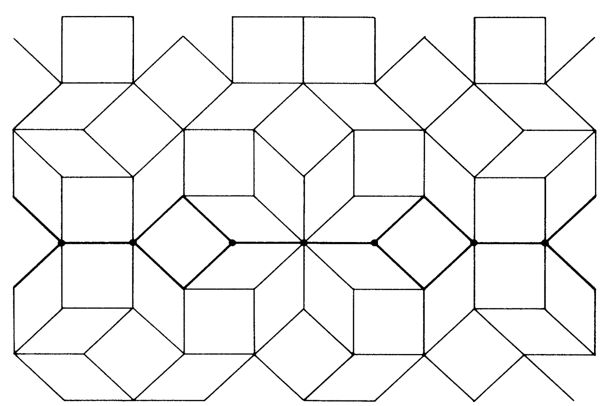

FIG. 1. A two-dimensional quasiperiodic tiling having octagonal point-group symmetry, which is also self-similar with respect to inflation and deflation transformations by a factor $1\pm\sqrt{2}$. Indicated in bold is a corresponding one-dimensional quasiperiodic pattern. The points indicated at the vertices define an octagonal chain.

generates a hyperbolic rotation by an angle $\phi = \ln(3+2\sqrt{2})$ having a trace equal to $2\cosh\phi = 6$, so that adopting the same notation as in the first example, the symbol of the multimetrical point group becomes

$$K = \{A,B,C,D\} = 4m\hat{6}\hat{m} \ . \tag{40}$$

Actually, the indefinite quadratic form $(1,-2,-1)$ associated to g_1 also admits negative units. A corresponding negautomorph transforms the metrical tensor g_1 into g_2, generates the inflation and deflation of the octogonal chain and can be expressed in terms of the generators already given:

$$F = ABC = \begin{bmatrix} 2 & 1 \\ 1 & 0 \end{bmatrix} = \check{2} \text{ so that } \tilde{F} g_1 F = -g_1 = g_2 \ . \tag{41}$$

By the symbol $\check{n}$ we indicate a negautomorph having determinant -1 and trace n.

It is convenient to make all of this explicit by using for this multimetrical point group instead of (40) the symbol

$$K = 4m\check{2}\hat{m} \tag{42}$$

and denoting the corresponding symmorphic multimetrical space group by

$$G = p4m\check{2}\hat{m} \ . \tag{43}$$

Of course, (40) and (42) indicate the same point group expressed in terms of a different set of generators.

It is interesting to note that the Euclidean fourfold rotation is at the same time an automorph of the positive definite quadratic form $g_0 = (1,0,1)$ and a negautomorph of the indefinite quadratic form $g_1 = (1,-2,-1)$:

$$E = AB = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \text{ with } \tilde{E} g_1 E = -g_1 \ . \tag{44}$$

This expresses one of the hidden relations between positive definite and indefinite binary integral quadratic forms.

In Fig. 2 one finds a simple point pattern having the multimetrical space group (43) as symmetry. In Fig. 3 it is shown how by strip-projection one gets from this pattern a decorated one-dimensional octagonal tiling, which admits an inflation/deflation rule (Fig. 4) with scaling factors $1 \pm \sqrt{2}$, which are the two eigenvalues of F. The corresponding scale-space group

$$G_{SR} = p\bar{1}\check{2}\hat{m} \tag{45}$$

is a subgroup of (43). In the example discussed in a previous paper,[14] the scale-space group $p\bar{1}\check{2}$ was considered instead, simply because non-Euclidean mirrors were disregarded.

C. A third example

A third example follows directly as a semidirect product of the lattice translation group Λ and the point group K considered in Sec. II C. It was obtained from the analysis of a two-dimensional superspace embedding on a square lattice of a Fibonacci chain.[11,14] Adopting the same conventions, one now has the following multimetrical point and space groups:

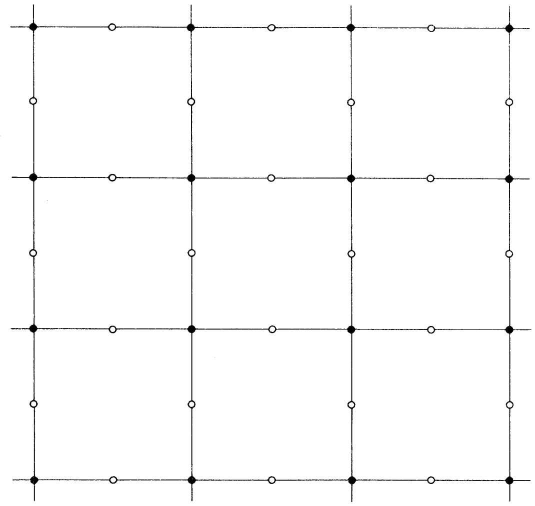

FIG. 2. A simple example of a crystallographic pattern having two-dimensional space-group symmetry $G_0 = p4m$, which is also invariant with respect to the multimetrical space group $G = p4m\check{2}\hat{m}$. It consists of two types of atoms, one at position a with coordinate 0,0 and another at position c with coordinates $\frac{1}{2}$,0 and 0,$\frac{1}{2}$ of the space group $p4m$, which is the Euclidean subgroup of G.

$$K = \{A,B,C,D\} = \{A,C,E,F\} = 4m\check{1}\hat{m}, \quad G = p4m\check{1}\hat{m} \tag{46}$$

with $4 = E = AB$, $m = A$, $\check{1} = F = ABC$, and $\hat{m} = C$.

V. RECIPROCAL SPACE

A. Reciprocal bases

Let us first introduce a basis $e_1^*, \ldots, e_n^*$ in the reciprocal multimetrical space V^* with compatible metric tensors g_ν^{0*}, dual with respect to the basis $e_1, \ldots, e_n$ previously considered for the direct space V, so that in matrix notation one has the relations:

$$g_\nu^0 g_\nu^{0*} = \mathbb{1}_n \quad \text{for } \nu = 1,2,\ldots,2^n \ . \tag{47}$$

Accordingly, the tensor components of the direct and of the reciprocal bases are correspondingly the same. The identification of V^* with V is done by means of the Euclidean scalar products (other choices being of course also possible and equivalent to the present one, but nevertheless different). Therefore, while we could take one direct basis $e_1, \ldots, e_n$ we now have to consider ν-dependent reciprocal bases (all being defined in V). Using the notation defined in Eq. (2) we have

$$e_i^*(\nu) = \epsilon_{\nu ii} e_i, \quad i = 1, \ldots, n \ , \tag{48}$$

so that for the Euclidean case one has

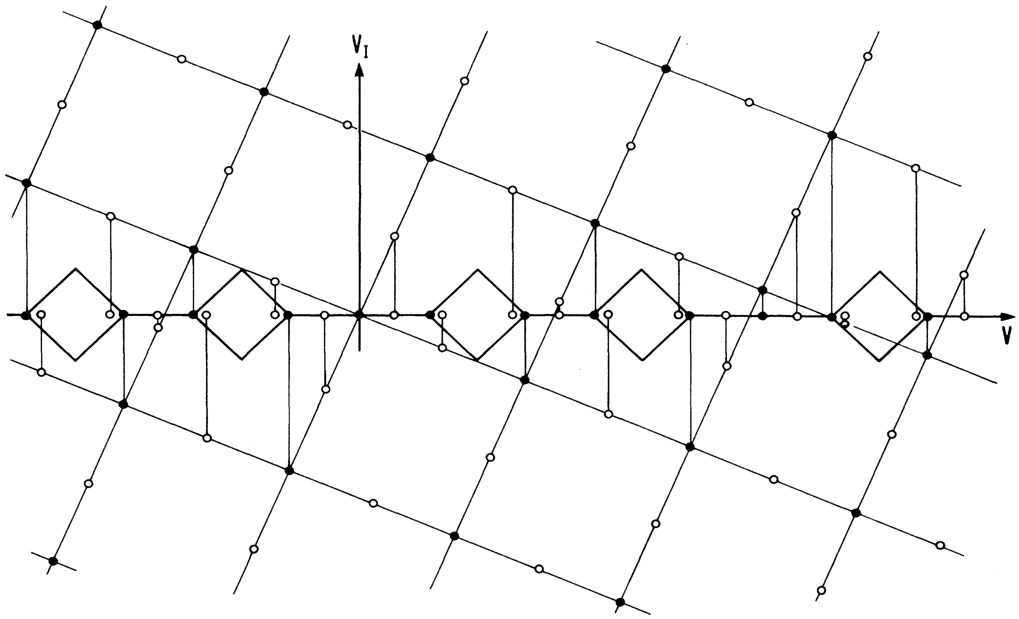

FIG. 3. The same pattern as in Fig. 2, if interpreted as being that of the two-dimensional superspace embedding of a one-dimensional quasiperiodic crystal, yields by projection on the physical space V of the atomic points within a given strip-region in superspace (one for each Wyckoff set and containing the so-called occupied positions), a decorated one-dimensional octagonal tilting. The squares indicated need not be part of the one-dimensional octagonal pattern. They are represented here for making the presence of two types of tiles more explicit.

$$e_i^* = e_i^*(0) = e_i \ . \tag{49}$$

Let us now consider the scalar product according to the various metrics of a reciprocal vector k with components k_i and of a direct vector x with components x_j. We have

$$k = \sum_{i=1}^{n} k_i e_i^*(\nu) \quad \text{and} \quad x = \sum_{j=1}^{n} x_j e_j \ . \tag{50}$$

One then verifies the relation

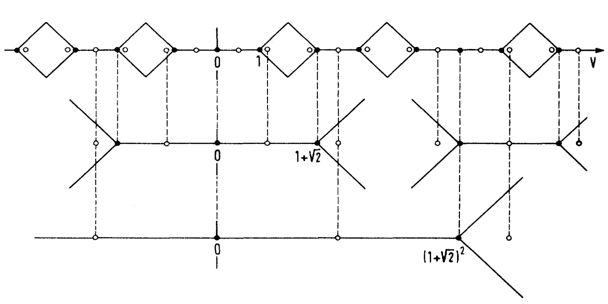

FIG. 4. The decorated tiling derived in Fig. 3 satisfies the same inflation and deflation rules as the original one based on the vertices only. It is (injectively) invariant with respect to the scale-space group $p\bar{1}\check{2}$ subgroup of the multimetrical group $p4m\check{2}\hat{m}$. Indicated are the deflations of the original pattern by scaling factors $1+\sqrt{2}$ and by $(1+\sqrt{2})^2$, respectively, and the corresponding pre-images. Note that this scaling symmetry requires a point-atom approximation of the structure.

$$k \overset{\nu}{\circ} x = \sum_{i=1}^{n} k_i x_i \ . \tag{51}$$

It has been already said, but it is important not to forget that after identification of V^* with V the components of k with respect to the basis $\{e_i\}$ of V are $\epsilon_{\nu ii} k_i$, and not k_i.

For clarifying further the multimetrical concept, let us take a concrete example: the one associated with the hexagonal lattice as discussed above in the first example. We have

$$a_1 = (1,0) = e_1, \quad a_2 = \left[\frac{1}{2}, \frac{\sqrt{3}}{2}\right] = \frac{1}{2} e_1 + \frac{\sqrt{3}}{2} e_2 \tag{52}$$

yielding, as in (28), the two metric tensors:

$$g_0 = \begin{bmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & 1 \end{bmatrix}, \quad g_1 = \begin{bmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{bmatrix} . \tag{53}$$

The dual bases for the reciprocal lattices Λ_ν^* in V^* have components

$$a_1^*(\nu) = e_1^*(\nu) - \frac{1}{\sqrt{3}} e_2^*(\nu), \quad a_2^*(\nu) = \frac{2}{\sqrt{3}} e_2^* \ . \tag{54}$$

After Euclidean identification of V^* with V, the dual basis for $\nu = 0$ becomes

$$a_1^*(0) = a_1^* = \left[1, -\frac{1}{\sqrt{3}}\right], \quad a_2^*(0) = a_2^* = \left[0, \frac{2}{\sqrt{3}}\right], \tag{55}$$

whereas for $\nu = 1$ it is given by

$$a_1^*(1)=\left[1,\frac{1}{\sqrt{3}}\right], \quad a_2^*(1)=\left[0,-\frac{2}{\sqrt{3}}\right], \tag{56}$$

ensuring duality $a_i \overset{\nu}{\circ} a_j^*(\nu)=\delta_{ij}$.

The metric tensor elements of $g^*(\Lambda)$ are, however, correspondingly the same for the two bases. Thus one can take as the reciprocal lattice Λ^* of the given Λ the one generated by the vectors a_1^* and a_2^* of the Euclidean dual basis and consider Λ^* generically as a lattice in the multimetrical space V, attaching to Λ^* a corresponding set of metric tensors $g(\Lambda^*)=\{g_\mu^*\}$.

In particular, for the example considered above, one has

$$g_0^*=\frac{4}{3}\begin{bmatrix}1 & -\frac{1}{2}\\ -\frac{1}{2} & 1\end{bmatrix} \quad \text{and} \quad g_1^*=\frac{4}{3}\begin{bmatrix}\frac{1}{2} & \frac{1}{2}\\ \frac{1}{2} & -1\end{bmatrix}. \tag{57}$$

One then verifies the duality condition in the form

$$g_0^* g_0 = \mathbb{1}_n \quad \text{and} \quad g_1^* g_1 = \mathbb{1}_n, \tag{58}$$

leading to invariance of the reciprocal lattice Λ^* for all multimetrical point-group transformations that leave Λ invariant. Indeed,

$$\tilde{A} g_\nu A = g_\mu \text{ implies } \tilde{A}^* g_\nu^* A^* = g_\mu^*, \tag{59}$$

where, as usual $A^* \equiv \tilde{A}^{-1}$. Therefore, to a point-group transformation A acting on a position vector x there corresponds one of $\tilde{A}$ acting on a reciprocal vector k, as one sees from Eq. (51). Indeed,

$$k \overset{\nu}{\circ} Ax = \sum_{i,j=1}^{n} k_i A_{ij} x_j = \tilde{A} k \overset{\nu}{\circ} x. \tag{60}$$

B. Structure factors

The point group of a multimetrical space group being, in general, infinite, one has to distinguish between two types of sets of equivalent points: those of finite multiplicity (within a lattice unit cell) and those of infinite multiplicity.

Typical for the situation is that a point in general position (having thus the identity of site symmetry) is of the second type, so that if the invariant pattern of a crystal consists of point-atoms, then these atoms are necessarily in special positions. The charge density (which does not satisfy that condition) will, normally speaking, not have equal value on equivalent points of infinite multiplicity. Therefore, we expect that if multimetrical symmetry appears in crystals, it will only apply to a crystal in the point-atom approximation and it will be broken by the presence of a continuous charge distribution. This does not mean that points of infinite multiplicity are necessarily irrelevant in crystal physics. Here, however, only positions of finite multiplicity will be considered.

The aim of this section is to show that the structure factor of a set of equivalent positions is invariant with respect to the multimetrical space group transformations so that such symmetries can in principle be detected from systematic extinctions in a diffraction pattern, as is the case for space and superspace groups.

Let us denote by r_0 a given atomic position and by $\{r_j, j=0,\ldots,s-1\}$ the corresponding set of equivalent positions within a given unit cell of the lattice Λ. That pattern admits a Euclidean description, which is at the basis of a diffraction experiment. Accordingly, in what follows the expressions involve Euclidean scalar products only, and the reciprocal lattice vectors H involved are elements of the Euclidean reciprocal lattice Λ^*. The non-Euclidean multimetric transformations acts as affine transformations and the corresponding point-group elements leave Λ^* invariant.

Putting the atomic scattering factor equal to 1, the structure factor takes the familiar form:

$$F(H)=\sum_{j=0}^{s-1} e^{2\pi i H r_j} = \sum_{A\in\{A_j\}} e^{2\pi i H[Ar_0+v(A)]}, \tag{61}$$

where the A_j are the coset representatives of the site symmetry group of r_0 in the point group K. Making use of the Frobenius congruence relations (21) and of Eq. (60), one verifies the invariance condition

$$F(\tilde{B}H)e^{2\pi i H v(B)}=F(H), \quad \text{any}\{B|a+v(B)\}\in G, H\in\Lambda^*, \tag{62}$$

expression which simplifies in the symmorphic case to:

$$F(\tilde{B}H)=F(H), \quad \text{for } G \text{ symmorphic and } B\in K. \tag{63}$$

VI. WYCKOFF POSITIONS

The number of Wyckoff positions of finite multiplicity is infinite, because there is an infinite number of different site symmetries. General expressions can be derived, but as that has not yet been done, it requires a fairly large amount of work even in the two-dimensional symmorphic cases. Therefore, only some few examples will be presented here in order to illustrate the concepts.

Before doing so, it is important to be aware of some basic properties characteristic for a multimetrical space group G with respect to the Wyckoff positions of the space group G_0, which is the subgroup of the Eulidean transformations belonging to G. As has already been pointed out, G_0, is, in general, of infinite index in G.

Two typical cases arise: (1) A set of equivalent positions with respect to G consists of whole sets of positions equivalent with respect to G_0. (2) A finite multiplicity set of equivalent positions is always a set of special positions, even if general with respect to the space group G_0.

Accordingly, one can possibly recognize the presence of multimetrical symmetries in a crystal seeking whether space-group-inequivalent Wyckoff positions are occupied by the same atomic species at a given Wyckoff position of a multimetrical space group. Furthermore, one can also look at atoms with coordinates not fixed by space-group symmetries, but fixed for a multimetrical space group. The corresponding coordinates then have to be stable within the same crystallographic phase.

In looking for these peculiarities, one has to take into account the fact that multimetrical symmetry may be broken in actual crystals, because of the presence of the continuous charge distribution.

As an example of the first situation, consider the symmorphic multimetrical space group $p4m\check{1}\hat{m}$ given in (46) as the third example of Sec. IV: then the set of fractional coordinates

$$0,\tfrac{1}{2};\quad \tfrac{1}{2},0;\quad \tfrac{1}{2},\tfrac{1}{2} \tag{64}$$

defines a Wyckoff position with site symmetry A,F^3,I, where I is the total inversion. With respect to the Euclidean subgroup $G_0=p4m$ this set splits into two different Wyckoff positions: $2c$ and $1b$, respectively, in the notation of the International Tables.[25]

The structure factor of the given set is

$$F(h,k)=e^{\pi i h}+e^{\pi i k}+e^{\pi i(h+k)}\ . \tag{65}$$

The invariance with respect to $p4m$ being evident, it is sufficient to consider the expressions transformed by the two generators C and D of the point group K as in (18). For C one has

$$\begin{aligned} F(h',k')&=F(h-k,-k)\\ &=e^{\pi i(h-k)}+e^{-\pi i k}+e^{\pi i(h-2k)}\ , \end{aligned} \tag{66}$$

and for D one has

$$\begin{aligned} F(h',k')&=F(h,-h-k)\\ &=e^{\pi i h}+e^{\pi i(-h-k)}+e^{-\pi i k} \end{aligned} \tag{67}$$

both expressions being indeed equal to $F(h,k)$, as required by Eq. (63).

As an illustration of the second situation, consider the set of equivalent positions for the multimetrical space group $p4m\check{2}\hat{m}$ of the second example of Sec. IV:

$$\tfrac{1}{4},\tfrac{1}{4};\quad \tfrac{3}{4},\tfrac{3}{4};\quad \tfrac{1}{4},\tfrac{3}{4};\quad \tfrac{3}{4},\tfrac{1}{4}\ , \tag{68}$$

with site symmetry C, F^4. It is a general position for the subgroup $p4m$ and a special position for the multimetrical space group. One can again explicitly test the invariance of the corresponding structure factor.

As a last example we take the case where the special position with respect to G fixes the value of a free parameter appearing in a Wyckoff position of the Euclidean subgroup G_0. Consider the multimetrical space group $p6m\hat{4}\hat{m}$ given in Sec. IV as a first example [see (35)]. The set of equivalent positions

$$\tfrac{1}{6},\tfrac{1}{6};\quad \tfrac{1}{3},\tfrac{5}{6};\quad \tfrac{5}{6},\tfrac{1}{6};\quad \tfrac{1}{6},\tfrac{2}{3};\quad \tfrac{2}{3},\tfrac{1}{6};\quad \tfrac{2}{3},\tfrac{1}{6}\quad \tfrac{5}{6},\tfrac{5}{6}\ . \tag{69}$$

has $m\hat{4}^2\hat{m}$ as the site symmetry group [see Eqs. (32) and (33) for the meaning of the generators.] This Wyckoff position is simply the $6e$ position of the space group $p6m$ for the value of the corresponding free parameter $x=\frac{1}{6}$. Note that here the setting $a\bar{b}$ has been used instead of the ab-type adopted by the International Tables.[25]

VII. CONCLUDING REMARKS

Multimetrical point and space groups seem to be interesting mathematical and geometrical objects. Whether or not they can be of relevance for crystals is not yet clear. One has typically a situation where concepts are required before an answer to that question can be given from an analysis of the large experimental data presently available on crystal structures. Some general criteria have been formulated for helping that investigation, but it is evident that too little is known on such a rich field for allowing, on the basis of what has been presented here, more than a superficial and limited exploration of the crystallographic data. Of course, the identification of even a single crystal structure having nontrivial multimetrical symmetry would be of great interest.

One expects that verifying the presence or absence of these symmetries in superspace embedded quasicrystals, giving rise in the physical space to space-scale transformations, should be easier than to do so for normal crystals, at least in the very few cases in which the structure of such quasicrystals have been determined, because then the inflation and deflation rules already impose severe restrictions. That investigation will certainly also help to clarify further what one can expect to find in crystals admitting multimetrical symmetries.

In any case, most relevant is the fact that crystallographic laws seem to apply in principle equally well in space and in superspace, and for commensurate as well as for incommensurate crystals. The field of crystallographic symmetries is currently wide open and promising.

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