substances have only few reflections, while at lower d values, where the density of peaks is higher, the proposed arrangement shows a much better resolution. The superior performance of the mosaic-crystal monochromator becomes even more evident if the resolution functions are compared to the limit that is set by the particle-size broadening from the sample. $\Delta d/d$ cannot exceed the value given by d/D where D is the thickness of the particle. In Fig. 10 a particle thickness of 1 μm was chosen. While the curve for the mosaic monochromator comes close to this limit the curves for the conventional optics and that of the particle-size limit diverge. The performance of the perfect-crystal monochromator is only better in the focusing minimum where it goes even below the particle-size limit.

Taking coarser grains is no real solution since then they could in principle be better investigated by single-crystal diffraction at a synchrotron-radiation source (Bachmann, Kohler, Schulz & Weber, 1985), avoiding overlapping reflections.

Concluding remarks

The resolution functions for different types of angle dispersive powder diffractometers in parallel-beam geometry have been calculated and compared with experimental values. It is shown that perfect-crystal monochromators at a low Bragg angle are not ideally suited to very high-resolution work although their performance is superior to diffractometers at conventional sources using focusing geometry. Therefore, a new arrangement employing mosaic crystals at angles close to backscattering is proposed, giving a resolution function close to the limit set by the particle-size broadening. Such an instrument would give the highest possible resolution that can be obtained with a polycrystalline sample.

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Which Symmetry Will an Ideal Quasicrystal Admit?

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(*Received* 14 *November* 1990; *accepted* 17 *April* 1991)

*A tribute in honour of Mrs C. H. MacGillavry**

Abstract

The crystallographic nature of a quasicrystal structure is expressed in terms of the possibility of labeling 'translationally' equivalent atomic positions by a set of n integers. The corresponding position vectors are integral linear combinations of n basic ones generating a vector module M of rank n and dimension m. Because of the aperiodic nature of the quasicrystal, n is larger than m. Typical values observed in nature

* Contribution based on a lecture delivered 8 December 1989 at the C. H. MacGillavry Symposium, Amsterdam.

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are $m=3$ and $n=5$ or $n=6$. Lattice symmetry is recovered by embedding the quasicrystal in an n-dimensional space (the superspace) in such a way that M is the projection of a lattice Σ. The rotational symmetries of the quasicrystal are included in those of the vector module M and, after embedding, appear as n-dimensional rotations leaving Σ invariant and a corresponding Euclidean metric. Scaling symmetries are also possible in the atomic point-like approximation of a quasicrystal. In that case, enlarging by a given constant factor all the distances between 'translationally' equivalent atoms, the 'inflated' pattern still belongs to the original one: the occupied atomic positions in space are transformed into other ones also occupied in the original structure. This is called inflation procedure (of a scaling invariant pattern), the reverse transformation being a deflation. The module M is then invariant with respect to such discrete dilatations. In the superspace these correspond to crystallographic point-group transformations leaving the lattice Σ and an indefinite metric invariant. Scaling symmetries in space appear as hyperbolic rotations in the superspace. In these non-Euclidean rotations the improper ones are included. The compatibility between the two types of n-dimensional point-group symmetries (Euclidean and non-Euclidean rotations) is discussed both at the level of the quasicrystal structure and of that of the double metrical nature of the translational lattice Σ. For a characterization of the symmetry of the quasicrystal, one eventually arrives at the concept of the scale-space group, which includes as its Euclidean subgroup an n-dimensional space group (the superspace group). Examples are taken from aperiodic tilings admitting inflation–deflation symmetry. The vertices of these tilings are supposed to represent 'translationally' equivalent atomic positions. A number of basic concepts not expected to be familiar to crystallographers, even if explained in the text, are also listed and defined in an Appendix.

1. Introduction

Caroline MacGillavry reveals in her work sensitivity to the beauty of geometrical symmetry seen through the mind at different levels. In her paper on M. C. Escher's graphic work there are three levels and she writes (MacGillavry, 1986):

'It is essential to distinguish between the two-dimensional symmetry of the print itself and the symmetry of the three-dimensional object it represents, and that of the image the print evokes in the mind'.

The aim of the present paper is to stress that quasicrystals are three-dimensional drawings by nature of higher-dimensional objects, which evoke in our minds the presence of still more symmetries and harmonies.

The present framework and the provisional character of the insights the author has on quasicrystal structures impose an exploratory character of an exposition based more on ideas and examples than on theory and proofs. In particular, elements of the octagonal quasicrystal phase (Kuo, 1987, 1990) will be used as illustration.

2. Indexing quasicrystal tilings

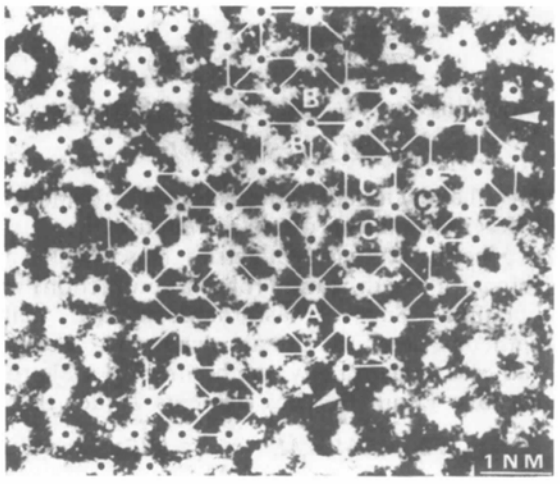
A geometrical description of a crystal in terms of atomic positions or of charge density can be done because of lattice translational symmetry, in terms of a unit cell which can be identified with a tile (the prototile) and of a filling of that unit cell, which then appears as a 'decoration' of the tile.

The theory of tilings (Grünbaum & Shepard, 1987), on the other hand, is much more general than that of monohedral periodic tiling (based on a single prototile) but most investigations are restricted to the two-dimensional case.

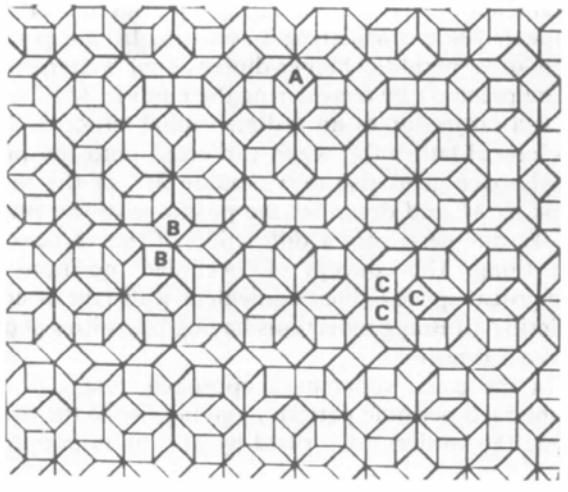
On the other hand, crystals are more general than simply periodic ones, as one knows after the discovery of incommensurate crystal structures, to which quasicrystals belong (see *e.g.* Janssen & Janner, 1987, and references therein). The description of their structure in terms of atomic positions and of charge density is much more involved than in the commensurate crystal case. Within the superspace approach, lattice periodicity is recovered by embedding the quasicrystal structure in a higher-dimensional space. The complexity is then hidden in the non-trivial relation between the Euclidean higher-dimensional crystallography and the original (lower-dimensional) structure.

The images one gets from high-resolution electron microscopy of quasicrystals are not directly interpretable in terms of atomic positions. Intriguingly enough, one recognizes a tiling structure compatible with the projection of part of the points of the higher-dimensional lattice of the embedded quasicrystal structure. It is essentially what one gets from the 'strip-projection method', where the strip describes the pre-image of the projected points. The strip is commonly the direct product of the physical space with the projection of a lattice unit cell on the orthogonal complement space, called internal space within the superspace approach.

Here very little will be assumed about that strip region except that it should give rise to an indexable tiling; this means that the position vectors of the vertices generate a free $\mathbb{Z}$ module $M \simeq \mathbb{Z}^r$. This is equivalent to a unique labeling (depending on the choice of the origin and of the basis) of those vertices by a finite set of integers $(n_1, n_2, \ldots, n_r)$. The dimension of M is that of the tiling, *i.e.* that of the real vector space generated by M, whereas the number r of free generators is the rank of M. Figs. 1 and 2 illustrate that situation for the case of the octagonal phase considered as two-dimensional quasicrystal



(*a*)



(*b*)

Fig. 1. High-resolution electron-micrograph image of the octagonal phase in Cr–Ni–Si alloy (*a*) and corresponding two-dimensional octagonal tiling (*b*). From a poster by K. H. Kuo distributed at the XIV IUCr Congress in Perth, Australia, 1987.

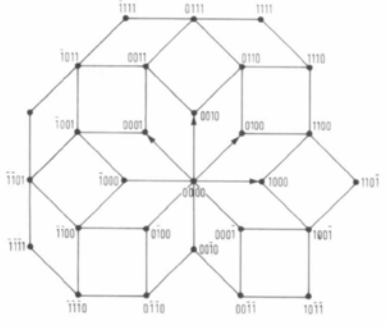


Fig. 2. Indexing of the vertices of the octagonal tiling of Fig. 1 according to a rank 4 vector module M with basis $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ and $\mathbf{a}_4$.

structure, which is periodic along the third dimension. The periodic direction will be disregarded. Fig. 1 illustrates the type of tiling observed in high-resolution electron-microscopy pictures. Fig. 2 indicates the corresponding indexing of the vertices according to a two-dimensional rank 4 module M generated by the vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$, $\mathbf{a}_4$.

The vertices are points at positions given by vectors $\mathbf{n}$:

$$\mathbf{n} = \sum_{i=1}^{4} n_i \mathbf{a}_i, \qquad \text{integers } n_i, \tag{2.1}$$

and define an octagonal tiling which is selfsimilar as illustrated in Fig. 3. In the corresponding inflation–deflation procedure the two prototiles Q (the square) and R (the rhombus) are transformed into inflated ones Q^* and R^*, respectively, according to the rule

$$Q^* = 3Q + 4R \quad \text{and} \quad R^* = 2Q + 3R \tag{2.2}$$

as one finds in Fig. 4. If one considers Q and R as free generators of a tile module, the corresponding transformation matrix T has eigenvalues given by the square of $\lambda_1 = 2^{1/2} + 1$ and $\lambda_2 = 2^{1/2} - 1$, where λ_1 and

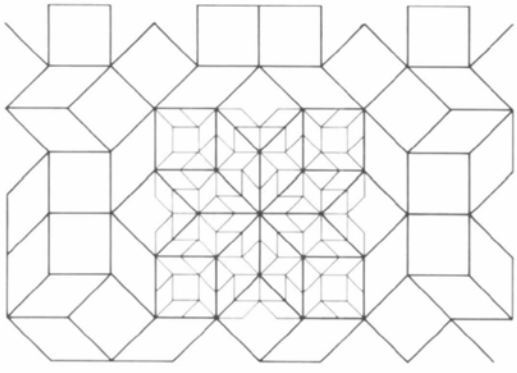


Fig. 3. Self-similarity of the octagonal tiling.

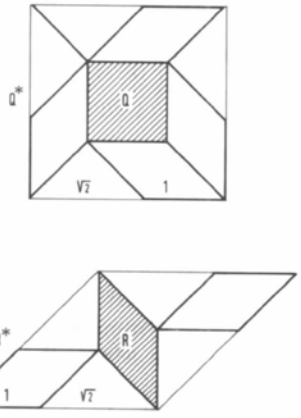


Fig. 4. Inflation–deflation rules for the prototiles Q (square) and R (rhombus).

λ_2 are the linear scaling factors for inflation and deflation, respectively;

$$T=\begin{pmatrix}3 & 2\\ 4 & 3\end{pmatrix}\sim\begin{pmatrix}2^{1/2}+1 & 0\\ 0 & 2^{1/2}-1\end{pmatrix}^2. \qquad (2.3)$$

The possibility of having an inflation-deflation rule is based on a scaling invariance of the vector module M underlying the pattern and is, accordingly, expressible as automorphism S of M, *i.e.* as 4×4 integral invertible matrix $\Gamma(S)$ when referred to the basis $\mathbf{a}_1,\ldots,\mathbf{a}_4$:

$$S\mathbf{a}_i=\sum_{j=1}^{4}\mathbf{a}_j\Gamma_{ji}(S)=\lambda\mathbf{a}_i. \qquad (2.4)$$

As one can read from Fig. 5, the scaling matrix describing dilatation by a scaling factor $\lambda=2^{1/2}+1$ is given by

$$\Gamma(S)=\begin{pmatrix}1 & 1 & 0 & \bar{1}\\ 1 & 1 & 1 & 0\\ 0 & 1 & 1 & 1\\ \bar{1} & 0 & 1 & 1\end{pmatrix}. \qquad (2.5)$$

The same tiling also admits rotational symmetries generated by a 45° rotation R_1 and a mirror R_2. Again, that is due to a rotational invariance of the vector module M:

$$R\mathbf{a}_i=\sum_{j=1}^{4}\mathbf{a}_j\Gamma_{ji}(R),\qquad R\in O(2), \qquad (2.6)$$

with $\Gamma(R)$ integral invertible (Fig. 6). The matrices expressing R_1 and R_2 are then given by

$$\Gamma(R_1)=\begin{pmatrix}0 & 0 & 0 & \bar{1}\\ 1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\end{pmatrix}$$

and (2.7)

$$\Gamma(R_2)=\begin{pmatrix}0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0\\ 0 & 1 & 0 & 0\\ 1 & 0 & 0 & 0\end{pmatrix}.$$

Note that in both cases the converse is not true: we mean by this that rotational and scaling invariance of M do not imply a corresponding symmetry of the tiling. Indeed, the module M describes *possible* positions, whereas the vertices of tiling consist of the *occupied* positions only. Of course, one can restrict considerations to the symmetries of the tiling only. In the spirit of Caroline MacGillavry, however, it is essential to take into account the symmetries of the underlying vector module M also.

For M we have identified two holohedral point groups, a rotational one H_R with elements R of $O(2)$ such that

$$RM=M,\qquad R\in O(2) \qquad (2.8)$$

and a scaling one H_S with elements S as above:

$$SM=\lambda(S)M=M \qquad (2.9)$$

with $\lambda(S)$ a real number different from zero and from one, describing thus a discrete dilatation.

In general, scaling symmetries may involve the combination of a dilatation (or of a contraction) with a rotation. Such transformations are called homotheties, the rotational symmetries being a special case. Accordingly, the holohedral scale-rotational point group H_{SR} has elements T such that

$$TM=\lambda M=M,\qquad T\in H(2), \qquad (2.10)$$

with $H(2)$ the group of homotheties of the two-dimensional space. As $O(2)$ is a subgroup of $H(2)$, so also H_R is one of H_{SR}.

Still another level of hidden symmetries of the tiling appears while considering it as arising from a projection of a periodic higher-dimensional pattern and more precisely by considering the module M of rank n as a projection of an n-dimensional lattice Σ. The reciprocal-lattice Σ^* when projected onto the physical space gives rise to a module M^* of the same rank as M and describes the positions of the Bragg peaks one gets from a diffraction of the vertices of the tiling. The concept of 'occupied' positions in reciprocal space is then equivalent with that of considering all Bragg reflections having intensities above a given threshold.

In the usual superspace approach, one gets the embedded periodic pattern ρ_s giving rise to the tiling (here the vertices) described by $\rho(r)$ by interpreting

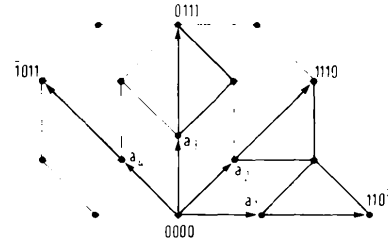


Fig. 5. Scaling symmetry of the vector module M underlying the inflation-deflation invariance of the octagonal tiling.

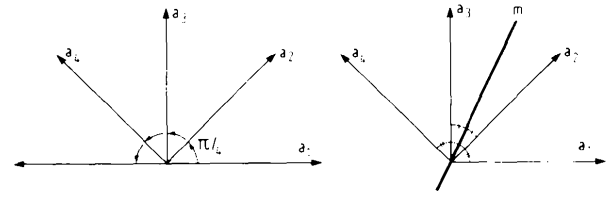


Fig. 6. Rotational symmetry transformations of the vector module M of the octagonal tiling.

the Fourier components of the two-dimensional tiling as those of an n-dimensional periodic one:

$$\rho(r) \overset{FT_2}{\leftrightarrow} \hat{\rho}(h_1, \ldots, h_n) \equiv \hat{\rho}_s(h_1, \ldots, h_n) \overset{FT_n}{\leftrightarrow} \rho_s(r_s) \tag{2.11}$$

where FT_n denotes the n-dimensional Fourier transform. Because M^* is the projection of Σ^*, one gets the vertices as intersection of the lines appearing in the pattern ρ_s with the physical space

$$\rho(r) = \rho_s(r_s) \cap V. \tag{2.12}$$

Analogous considerations apply to the three-dimensional (or to the one-dimensional) quasicrystal case. In the present analysis the vertices are projections of lattice points in the higher-dimensional space. The two approaches based on projection, the one in reciprocal space and the other in direct space, are equivalent because the structure in physical space is the same, but they are different: points are not lines. To avoid misunderstanding we will call the present one a direct superspace approach (Janner, 1989, 1990*a*; Janner & Janssen, 1990), as opposed to the usual (reciprocal) superspace description.

3. Superspace embedding

Let us first consider the one-dimensional octagonal chain one gets by restriction to the vertices of the octagonal tiling lying on a line V^0 parallel to $\mathbf{a}_1$, which can be considered to describe a one-dimensional quasicrystal. These vertices are at positions (Fig. 7)

$$\mathbf{n} = n_1\mathbf{b}_1 + n_2\mathbf{b}_2$$

with

$$\mathbf{b}_1 = \mathbf{a}_1 \quad \text{and} \quad \mathbf{b}_2 = (1+2^{1/2})\mathbf{a}_1 \tag{3.1}$$

and are thus indexed by two integers n_1, n_2, so that the occupied positions generate a set of possible ones and define a vector module M^0 of dimension 1 and of rank 2. Embedding in superspace is possible on a square lattice Σ^0 (see Fig. 8) with basis vectors

$$\mathbf{b}_{1s} = (\mathbf{b}_1, \mathbf{b}_2) \quad \text{and} \quad \mathbf{b}_{2s} = (\mathbf{b}_2, -\mathbf{b}_1). \tag{3.2}$$

The first components along V^0 generate M^0. The second ones generate another $\mathbb{Z}$ module, as considered below, which spans the one-dimensional space V_I^0 (called internal) orthogonal to V^0. The embedding chosen is such that the basis vectors $\mathbf{b}_{1s}$ and $\mathbf{b}_{2s}$ in the superspace $V_s = V^0 \oplus V_I^0$ have the same length. So the metric tensor of the basis (3.2) is given by

$$g_e^0 = 2(2+2^{1/2})a_1^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{3.3}$$

In Fig. 9 the lattice points are indicated which correspond to the occupied positions leading by projection to the atomic arrangement at the vertices of a (dihedral) tiling with prototiles $\mathbf{b}_1$ and $\mathbf{b}_2$. The scaling symmetry of M^0 is expressed by the inflation-deflation rule with scaling factors $2^{1/2}+1$ or $2^{1/2}-1$. In the same way as in (2.2) we now have

$$A^* = B, \qquad B^* = A + 2B \tag{3.4}$$

with $A = |\mathbf{b}_1|$ and $B = |\mathbf{b}_2|$.

The corresponding scaling transformation S is expressed by the same integral matrix, both with respect to the basis $\mathbf{b}_1$, $\mathbf{b}_2$ of M^0 and to the basis $\mathbf{b}_{1s}$, $\mathbf{b}_{2s}$ of Σ^0, having determinant -1, trace 2 and eigenvalues $1 \pm 2^{1/2}$:

$$\Gamma(S) = \begin{pmatrix} 0 & 1 \\ 1 & 2 \end{pmatrix} \sim \begin{pmatrix} 1+2^{1/2} & 0 \\ 0 & 1-2^{1/2} \end{pmatrix} = \begin{pmatrix} e^{\chi} & 0 \\ 0 & -e^{-\chi} \end{pmatrix} \sim \begin{pmatrix} \sinh\chi & \cosh\chi \\ \cosh\chi & \sinh\chi \end{pmatrix} \tag{3.5}$$

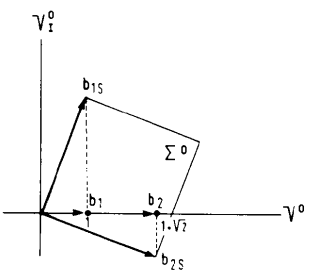


Fig. 8. Superspace embedding of the rank 2 module M^0 on a two-dimensional lattice Σ^0, which in the present case is a square lattice.

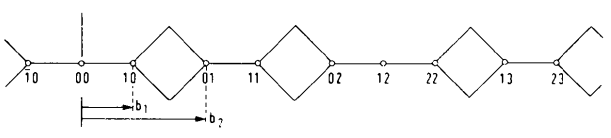


Fig. 7. A one-dimensional tiling generated by the vector module $M^0 = \{\mathbf{b}_1, \mathbf{b}_2\}$ with vertices belonging to those of the octagonal tiling along a given line.

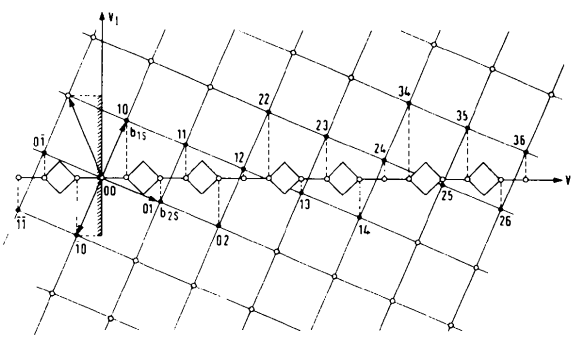


Fig. 9. Occupied lattice point positions giving by projection the vertices of the one-dimensional octagonal chain.

where $\sim$ means matrix equivalency by conjugation with elements of $Gl(2,\mathbb{R})$. The relation

$$2\sinh\chi = 2 \tag{3.6}$$

corresponds to a (crystallographic) condition imposed on the last matrix transformation for leaving a two-dimensional lattice invariant. In order to obtain a better understanding of the geometrical nature of S, once viewed as a superspace transformation, it is convenient to consider the two-dimensional Euclidean crystallography as a special case of a more general two-dimensional one, where the space is a plane admitting indefinite metric tensors also.

4. Two-dimensional metrical crystallography

The present ideas were first developed within the framework of crystallography of space-time (Janner & Ascher, 1969*a*, *b*, *c*). Here a similar approach appears because of the possibility of embedding quasicrystal structures in a superspace having in addition to the Euclidean metric an indefinite metric as well. To deal with multimetrical spaces requires a more general crystallographic characterization than is usually adopted. This point of view is discussed in another paper (Janner, 1991). The motivation, however, is based on the need to admit scaling symmetries in addition to the normal crystallographic ones described by a space group and this is the main concern of the present paper. For this reason, some of the basic ideas of a multimetrical crystallography are presented here in the simple two-dimensional case. Before doing that, one needs to know at least some typical elements of non-Euclidean crystallography compared to the familiar Euclidean ones. As already discussed a number of years ago in the paper mentioned above (Janner & Ascher, 1969*a*), that is possible within a general framework which deals with crystallographic laws, without the need to specify beforehand the character of the metric involved.

The first basic concept is that of the symmetry of a lattice, expressed in terms of a holohedral point group leaving the lattice and an appropriate metric tensor invariant. A lattice is said to be isometric if it has a non-reducible point symmetry (*i.e.* referring the holohedral point group to a lattice basis gives rise to a non-reducible faithful integral representation). In that case the holohedral point group H contains a transformation R such that a lattice vector $\mathbf{a}$ and the transformed one $R\mathbf{a}$ generate the space, in this case the plane. The non-isometric lattices can be derived from a combination of lower-dimensional isometric ones.

The next concept is that of a natural lattice. A two-dimensional natural lattice is a particular isometric lattice which admits a basis $\mathbf{a}_1$ and $\mathbf{a}_2$ such that

$$\mathbf{a}_2 = R\mathbf{a}_1 \quad \text{for given} \quad R \in H. \tag{4.1}$$

All other isometric lattices of the same dimension then follow from an operation known as centering. This approach can be generalized to n dimensions allowing one to derive n-dimensional crystallography from an *Aufbauprinzip*.

If R is proper (det $R = 1$), then with respect to the basis (4.1) it takes the form

$$\Gamma(A_\mu) = \begin{pmatrix} 0 & -1 \\ 1 & \mu \end{pmatrix}, \qquad \text{integer } \mu, \tag{4.2}$$

and the corresponding natural lattice is denoted by M_μ. If det $R = -1$, then for the same basis it is given by

$$\Gamma(N_\nu) = \begin{pmatrix} 0 & 1 \\ 1 & \nu \end{pmatrix}, \qquad \text{integer } \nu, \tag{4.3}$$

and the natural lattice is indicated by Λ_ν. In both cases a metric tensor of the basis $\mathbf{a}_1$, $R\mathbf{a}_1$ can be defined according to

$$g_\mu = \begin{pmatrix} 1 & \mu/2 \\ \mu/2 & 1 \end{pmatrix} \quad \text{and} \quad g_\nu = \begin{pmatrix} 1 & \nu/2 \\ \nu/2 & -1 \end{pmatrix}, \tag{4.4}$$

the corresponding binary integral quadratic form being denoted by

$$(1, \mu, 1) \quad \text{and} \quad (1, \nu, -1), \tag{4.5}$$

respectively. Then A_μ is an automorph of g_μ and N_ν a negautomorph of g_ν. Indeed one verifies the relations

$$\tilde{\Gamma}(A_\mu) g_\mu \Gamma(A_\mu) = g_\mu \quad \text{and} \quad \tilde{\Gamma}(N_\nu) g_\nu \Gamma(N_\nu) = -g_\nu, \tag{4.6}$$

where the tilde means transposition, so that N_ν^2 is also an automorph of the quadratic form of g_ν. The quadratic forms (4.5) are positive definite for $|\mu| < 2$ and indefinite for $|\nu| > 0$ and for $|\mu| > 2$ (Figs. 10 and 11). The $|\mu| = 2$ case corresponds to the parabolic one

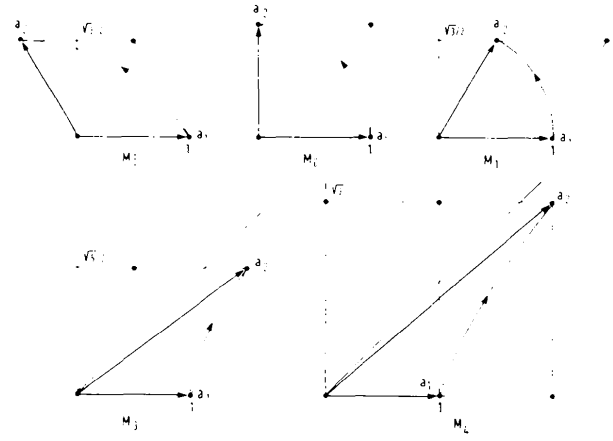


Fig. 10. Natural lattices of the type M_μ for values of $\mu = -1$, 0, 1, 3 and 4.

and $\nu = 0$ is also a special case. In the indefinite metrical case, one easily constructs the lattices M_μ and Λ_ν in the following way. Consider an orthonormal coordinate system with basis vectors $\mathbf{e}_1$ and $\mathbf{e}_2$ along the 'space' direction x and along the 'time' direction ct, respectively. Using for the lattice M_μ the crystallographic condition $2\cosh\chi = \mu$, (4.1) with $\mathbf{a}_1 = a\mathbf{e}_1$ becomes $\mathbf{a}_2 = (a/2)[\mu\mathbf{e}_1 + (\mu^2-4)^{1/2}\mathbf{e}_2]$. In the same way for Λ_ν with $\nu = 2\sinh\chi$, one gets correspondingly $\mathbf{a}_2 = (a/2)[\nu\mathbf{e}_1 + (\nu^2+4)^{1/2}\mathbf{e}_2]$. Thus, in the Euclidean representation, these lattices are rectangular for μ, ν even and rhombic for μ, ν odd.

The interest in this general approach is that crystallographic laws become more transparent because they are valid for arbitrary values of the integers μ and ν and are not restricted to a finite number of cases (like in the hexagonal and square lattice cases) as occurs in Euclidean crystallography.

As an example, consider the set of points invariant with respect to a point-group transformation A_μ, having thus A_μ as stabilizer. They form a lattice denoted by $M_{\mu,1}$ which contains M_μ as a sublattice. (The same is correspondingly the case for N_ν, $\Lambda_{\nu,1}$ and Λ_ν.) Then one finds the general law

$$\text{index}\,(M_\mu \subset M_{\mu,1}) = |\mu - 2| \quad \text{and} \quad \text{index}\,(\Lambda_\nu \subset \Lambda_{\nu,1}) = |\nu|. \tag{4.7}$$

This situation is depicted in Fig. 12 for low values of μ and ν. For $\mu = -1$, 0, 1, one recognizes the well known Euclidean cases as obtained from the Cheshire symmetry (Hirshfeld, 1968) of the corresponding space groups $p3$, $p4$ and $p6$. We recall that the Cheshire group of a space group is its normalizer in the Euclidean group of the same dimension (Wondratschek, 1983).

In the same way, the points having an A_μ^k site symmetry belong to a lattice $M_{\mu,k}$ and those with N_ν^k site symmetry to a lattice $\Lambda_{\nu,k}$. For those lattices analogous general laws can be formulated.

Considering again the generator (3.5) of the scaling transformation of the one-dimensional octagonal case, one recognizes the relation

$$\Gamma(S) = \Gamma(N_2), \qquad i.e.\ S = N_2. \tag{4.8}$$

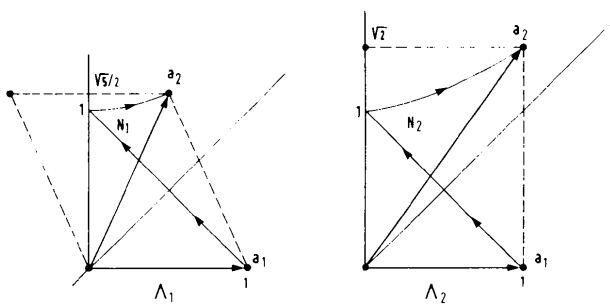


Fig. 11. Natural lattices of the type Λ_ν for the values $\nu = 1$ and 2.

Indeed, identifying the physical one-dimensional space V^0 with one branch of the light cone and the internal space V_I^0 with the other branch, one sees that to a discrete dilatation in V^0 by e^x there corresponds a contraction by $-e^{-x}$ in V_I^0, the invariance of the lattice being ensured by the integral condition (3.6) (Fig. 13). Note that the lattice, generated by the basis (3.2), is a square one (from the Euclidean point of view), whereas this is not the case for Λ_2 as represented in Fig. 11. The two lattices are actually equivalent and only differ in the choice of the reference system.

Change of the reference system does not change the symmetry of a lattice: that is here also the case if one takes into proper account the metrical aspects. Consider

$$S = N_2 \in IO(1,1) \tag{4.9}$$

where $IO(1,1)$ is generated by the orthogonal group $O(1,1)$ isomorphic to the two-dimensional Lorentz

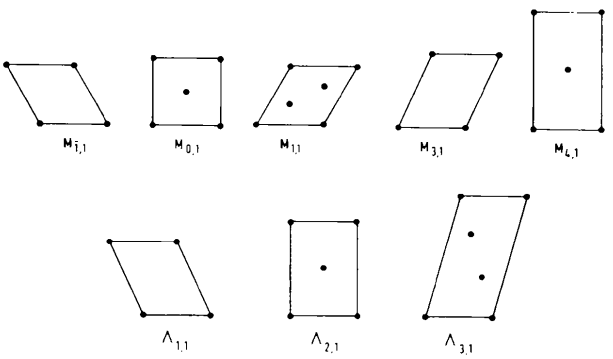


Fig. 12. Symmetry elements A_μ of the corresponding lattices M_μ for $\mu = -1$, 0, 1, 3 and 4. The same for the symmetry elements N_ν and the lattices Λ_ν for $\nu = 1$, 2 and 3.

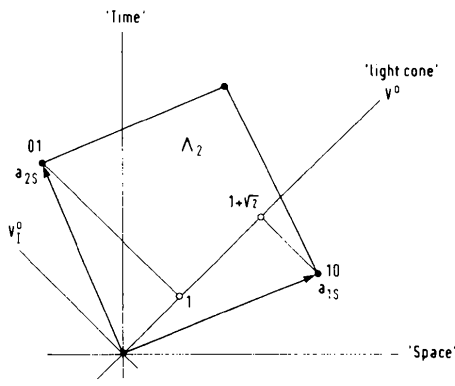


Fig. 13. Orientation in the indefinite metric plane (with respect to the 'space' and 'time' axes) of the square lattice giving by projection of the occupied positions the one-dimensional octagonal chain. (With respect to the corresponding Figs. 8 and 9 one has $\mathbf{b}_{2\perp} = \mathbf{a}_{1\perp}$ and $\mathbf{b}_{1\perp} = \mathbf{a}_{2\perp}$.) The scaling matrix is now $\Gamma'(N_2) = \begin{pmatrix} 2 & 1 \\ 1 & 0 \end{pmatrix}$.

group and the transformation I which interchanges 'time' and 'space' axes. A conjugation of S by an element T of $IO(1,1)$ corresponds to a change of reference system in the indefinite metric plane and does not change what we may call the scaling holohedry, but changes, of course, the metrical properties of $\Sigma^0 = \Lambda_2$ when considered as a lattice in the Euclidean plane. The process of transforming Λ_2 by such a change of the indefinite metric frame to a lattice Σ^0 isometric with respect to an Euclidean metric is called *Euclidization.*

Fig. 14 illustrates the process of Euclidization for the lattice Λ_2 transforming it to the Euclidean square lattice (see for comparison Figs. 11 and 13). Fig. 15 illustrates the same process for the lattice Λ_1 $(=M_3)$, also transformed into a square lattice M_0 $(=\Lambda_1)$.

The possibility of Euclidization illustrates hidden relations between Euclidean and non-Euclidean crystallography. The examples given are representative ones, in the sense that the same property is true in an infinite number of cases. Indeed, one has for example

$$M_{3,k} \overset{c}{\simeq} M_0 \quad \text{any} \quad k \in \mathbb{Z}. \tag{4.10}$$

This relation simply says that the set of points

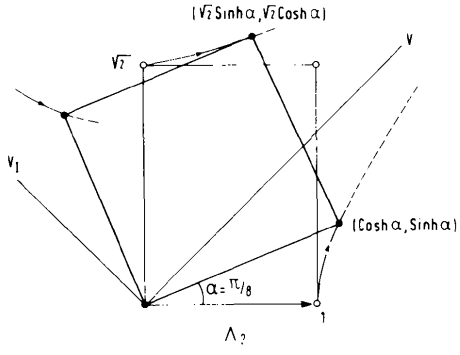


Fig. 14. Euclidization of the scaling invariant lattice Λ_2 from a rectangular to a square lattice.

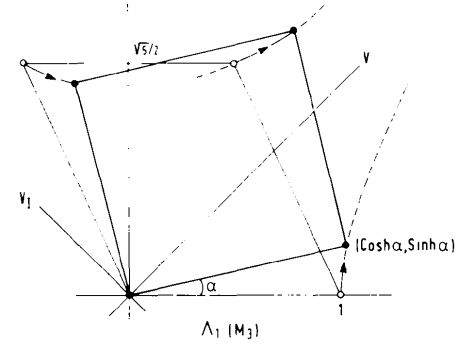


Fig. 15. Euclidization of the scaling invariant lattice Λ_1 (which coincides with M_3). It is transformed from a rhombic to a square lattice by changing the reference frame.

invariant with respect to a given scaling transformation

$$A_3^k \sim \begin{pmatrix} 0 & -1 \\ 1 & 3 \end{pmatrix}^k \sim \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix}^k$$

form a square lattice in an appropriate reference system.

From an intuitive point of view, one understands well that the scaling properties of a given tiling (*e.g.* the octagonal one) are not independent of the rotational symmetries of the same tiling (the eightfold symmetry in the octagonal case). Euclidization is a technical means for making such a relation more explicit.

Euclidization represents the deeper level where new symmetries become apparent, as mentioned at the end of § 2. In the next section, that level of hidden symmetries in quasicrystals will be investigated further, always in the spirit of Caroline MacGillavry.

5. Towards an optimal superspace embedding

The embedding of a vector module M on a lattice Σ in superspace is not unique even if one-to-one in the case that the dimension of the superspace is equal to the rank of M. Indeed, lattices having the same projection on the physical space are equivalent with respect to the structure of the quasicrystal.

This does not mean that all possible embeddings are equally well adapted from the point of view of a symmetry description in superspace. As people, in general, find that point difficult to grasp, let us give some nearly self-evident examples of comparable situations.

First, the properties of a physical system are independent of the coordinate system adopted. Nevertheless, it makes a big difference if one works with symmetry-adapted coordinates or not. The most symmetric coordinate system, say an orthonormal one, is in general not symmetry adapted. So which is the best reference frame depends on the physical system and on the symmetries considered.

Second, the crystal potential is not unique. It is always possible to adopt a gauge such that the only Euclidean symmetry of the potential is the identity, but again that is inconvenient. One always chooses the potential having the largest Euclidean symmetry possible and for a crystal one normally takes one having the symmetry of a space group.

In the case of a superspace embedding, the situation is subtle because what optimal embedding really means is a symmetry-adapted one, but it is not *a priori* clear which symmetries one has to consider. This fact has already been suggested by the title of the present paper.

In what follows, we will assume that the relation between superspace and physical space is an

orthonormal projection (which one depends on whether the direct- or the reciprocal-space approach has been adopted). A non-orthogonal projection has been considered by Yamamoto (1990), but we are not yet able to discuss this possibility within the framework of the present paper.

The rank 2 case suffices for explaining the ideas and if not explicitly stated otherwise we will assume a Euclidean superspace.

5.1. *Direct and reciprocal vector modules*

Consider the following direct and reciprocal one-dimensional rank 2 vector modules:

$$M = \{\mathbf{a}_1, \mathbf{a}_2\} \quad \text{and} \quad M^* = \{\mathbf{a}_1^*, \mathbf{a}_2^*\}. \tag{5.1}$$

A general (orthogonal) superspace embedding on dual bases for the lattices Σ and Σ^*, respectively, has the form

$$\begin{aligned} \mathbf{a}_{1s} &= (\mathbf{a}_1, \mathbf{a}_{I1}) \qquad \mathbf{a}_{2s} = (\mathbf{a}_2, \mathbf{a}_{I2}) \\ \mathbf{a}_{1s}^* &= (\mathbf{a}_1^*, \mathbf{a}_{I1}^*) \qquad \mathbf{a}_{2s}^* = (\mathbf{a}_2^*, \mathbf{a}_{I2}^*). \end{aligned} \tag{5.2}$$

The projection on the first (external) components yields the generators of the two vector modules M and M^*. The projection on the second (internal) components generates two other vector modules (called internal):

$$M_I = \{\mathbf{a}_{I1}, \mathbf{a}_{I2}\} \quad \text{and} \quad M_I^* = \{\mathbf{a}_{I1}^*, \mathbf{a}_{I2}^*\}. \tag{5.3}$$

Duality between the two bases of (5.2) implies the interesting relation:

$$M_I \approx M^* \quad \text{and} \quad M_I^* \approx M, \tag{5.4}$$

where two modules only differing by a constant factor are considered to be equivalent. This relation explains many of the crystallographic peculiarities of the internal space *versus* the external one, for both direct and reciprocal spaces.

The point is now that, if one adopts the standard embedding used for modulated crystal structures, where $\mathbf{a}_1^*$ generates the main reflections (here in one dimension) and $\mathbf{a}_2^* = \mathbf{q}$ is the modulation wave vector, one has

$$\begin{aligned} \mathbf{a}_{1s} &= (\mathbf{a}_1, -(\mathbf{a}_1 \cdot \mathbf{q})\mathbf{d}) \qquad \mathbf{a}_{2s} = (0, \mathbf{d}) \\ \mathbf{a}_{1s}^* &= (\mathbf{a}_1^*, 0) \qquad \mathbf{a}_{2s}^* = (\mathbf{a}_2^*, \mathbf{d}^*). \end{aligned} \tag{5.5}$$

Note that now $\mathbf{a}_2$ vanishes, so that M is no longer a rank 2 module. In this case one would never recognize the existence of a duality relation between internal and external space. The meaning of M for a modulated structure is clear, but its relevance obscure, whereas in the case of a quasicrystal M plays an important role. For quasicrystals, the choice of the embedding (5.5) is not justified, from both the experimental and the conceptual points of view, because there is no separation into a lattice of main reflections and a set of additional satellite reflections.

5.2. *Isometric lattice embedding: Euclidization*

As already stressed in previous papers (Janner, 1986, 1988, 1989) and illustrated by the example of a superspace embedding of a Fibonacci chain on a square lattice, it is always possible to embed a high-symmetry vector module on a less-symmetric lattice, but the converse is not true. In particular, embedding on isometric lattices Σ and Σ^* giving by orthogonal projection the vector modules M and M^*, respectively, imposes restrictions. For understanding the structural meaning of the non-reducible point-group elements of the holohedry of an isometric lattice additional concepts are needed.

In particular, concepts like 'multimetrical space' and 'Euclidization' represent a key for further understanding. A full treatment of these concepts lies beyond the aim of the present paper. Only some basic ideas will be presented here, together with some simple cases as illustration.

Consider a quasicrystal with a vector module M admitting both a rotational holohedry H_R and a scaling holohedry H_S, the latter being based on the invariance with respect to an indefinite metric tensor for the lattice Σ on which M has been embedded. Change of the orientation of the lattice within the indefinite space by means of a corresponding indefinite orthogonal transformation does not change the scaling holohedry, as already mentioned. Such a transformation, however, changes in general the Euclidean holohedry of Σ.

The process of finding for given H_S of M the largest Euclidean holohedry for Σ is the Euclidization of the scaling invariant lattice introduced in the previous section.

In that way, indefinite rotations become related to Euclidean ones which, under appropriate conditions, appear to be the non-reducible point-group elements mentioned above. A concrete example which applies to the superspace embedding of an octagonal chain can help to understand the situation.

The scaling matrix $\Gamma(S)$ of (3.5) is according to (4.8) a negautomorph of the indefinite quadratic form $(1, 2, \bar{1})$ defining a natural lattice Λ_2. In the standard orientation, one of the basis vectors lies along the 'space' direction and the second one can be chosen along the 'time' axis (as one can see from the quadratic form given above), so that Λ_2 appears in what we may call the 'rest frame'. From a Euclidean point of view, Λ_2 is then a rectangular lattice spanned by $\mathbf{e}_1 = (1, 0)$ and $2^{1/2}\mathbf{e}_2 = (0, 2^{1/2})$. Conjugation by

$$L = \begin{pmatrix} \cosh\alpha & \sinh\alpha \\ \sinh\alpha & \cosh\alpha \end{pmatrix}$$

with

$$\tanh\alpha = 2^{1/2} - 1 \tag{5.6}$$

transforms the lattice vectors $(1, 0)$ and $(-1, 2^{1/2})$ of

Λ_2 into

$$\mathbf{a}_{1s} = \cosh\alpha(1, \tanh\alpha),$$
$$\mathbf{a}_{2s} = \cosh\alpha(2^{1/2}\tanh\alpha - 1, 2^{1/2} - \tanh\alpha). \tag{5.7}$$

With respect to a Euclidean orthonormal basis, these same components define now a square lattice as in (3.2). The lattice is still Λ_2, but in another reference frame, as depicted in Fig. 14. Accordingly, the transformation (5.6) represents the Euclidization of the lattice Λ_2. In some cases, the Euclidization can be trivial, as is the case for the natural lattice M_4 which in the centered form $M_{4,1}$ is already hexagonal in its 'rest frame' (see Figs. 10 and 12). In Fig. 15 the Euclidization is shown of the lattice Λ_1, which is at the same time also that of M_3: a rhombic lattice as it appears in the 'rest frame' is transformed to a square lattice in the 'moving frame' with rapidity $\tanh\alpha = 5^{1/2} - 2$. The existence of a Euclidization does not mean that it is unique.

In order to see in an example the meaning of what has been said about the compatibility between isometric rotations and scaling, consider the scaling transformation N_2, which is a symmetry of the lattice Λ_2, now with respect to the square-lattice basis given in (5.7), which is related to the original one of (4.1) by

$$\mathbf{a}_{1s} = \mathbf{a}_1, \qquad \mathbf{a}_{2s} = \mathbf{a}_2 - 2\mathbf{a}_1. \tag{5.8}$$

Therefore, the scaling transformation N_2 is now represented by the matrix $\Gamma'(N_2)$:

$$\Gamma'(N_2) = \begin{pmatrix} 1 & 2 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 2 \end{pmatrix}\begin{pmatrix} 1 & -2 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 2 & 1 \\ 1 & 0 \end{pmatrix}. \tag{5.9}$$

One then verifies that it transforms (modulo Σ^0) the point $(\frac{1}{2}, 0) = \frac{1}{2}\mathbf{a}_{1s}$ into the point $(0, \frac{1}{2}) = \frac{1}{2}\mathbf{a}_{2s}$, whereas it leaves the point $(\frac{1}{2}, \frac{1}{2})$ invariant, in the same way as is achieved by a rotation of $\pi/2$.

Of course, much more has to be said about such hidden relations between Euclidean and non-Euclidean crystallographic transformations in order not to be misleading.

The validity of the considerations made is not restricted to the rank 2 case, as one can see from a multimetrical embedding of the rank 4 module of the octagonal tiling considered in § 2.

The superspace embedding of the four generators of the vector module M indicated in Fig. 2 is given, with respect to a Euclidean orthonormal basis, by

$$\mathbf{a}_{1s} = (1, 0, 1, 0) \qquad \mathbf{a}_{2s} = 2^{-1/2}(1, 1, -1, 1)$$
$$\mathbf{a}_{3s} = (0, 1, 0, -1) \qquad \mathbf{a}_{4s} = 2^{-1/2}(-1, 1, 1, 1) \tag{5.10}$$

and the Euclidean metric tensor is that of a hypercubic lattice:

$$g_e = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}. \tag{5.11}$$

One verifies that indeed the generators of the rotational point group H_R indicated in (2.7) leaves this metric tensor invariant.

The orientation of the same set of basis vectors $\mathbf{a}_{1s}, \ldots, \mathbf{a}_{4s}$ with respect to an indefinite orthonormal metric tensor with diagonal elements $(\bar{1}, \bar{1}, 1, 1)$ is then

$$\mathbf{a}_{1s} = 2^{1/2}[0, 0, 1, 0] \qquad \mathbf{a}_{2s} = [1, 1, 0, 0]$$
$$\mathbf{a}_{3s} = 2^{1/2}[0, 0, 0, 1] \qquad \mathbf{a}_{4s} = [\bar{1}, 1, 0, 0] \tag{5.12}$$

and again the lattice is hypercubic, but now according to the indefinite metric tensor

$$g_i = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & -2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & -2 \end{pmatrix}. \tag{5.13}$$

One can now also verify that the scaling matrix given in (2.5) is a negautomorph:

$$\tilde{\Gamma}(S) g_i \Gamma(S) = -g_i, \tag{5.14}$$

equivalent to the corresponding rank 2 transformation $N_2 \oplus N_2$.

In the present case, the relation between the indefinite orthonormal basis vectors $[1, 0, 0, 0], \ldots, [0, 0, 0, 1]$ and the two-dimensional sublattices Λ_2 arises as a combination of $\mathbf{a}_{1s}$ and $\mathbf{a}_{3s}$, respectively, and the centering of the square lattice generated by $[1, 0, 0, 0]$ and $[0, 1, 0, 0]$.

The various shapes occurring in the octagonal tiling represent the projection of three-dimensional faces of four-dimensional hypercubes (Fig. 16).

6. Scale-space groups for quasicrystals

The concept of scale-space groups was introduced by Janner & Janssen (1990) and considered further by Janner (1990*a*, *b*) and Janssen (1990).

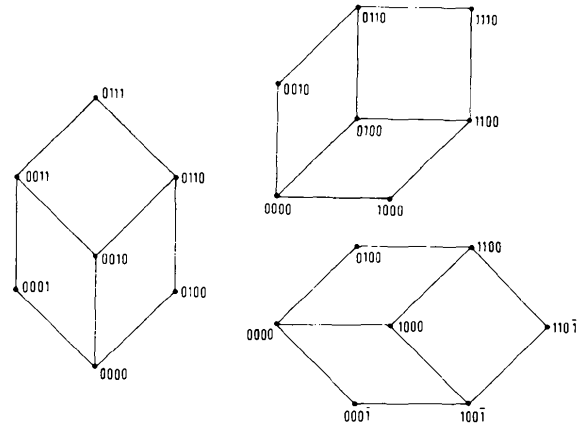


Fig. 16. Three-dimensional faces of hypercubes appearing in the octagonal tiling from a projection on the plane of points of a cubic lattice in four dimensions.

In § 2, the holohedral scale-rotational point group H_{SR} of a given vector module M of rank n has been introduced. On a basis $\mathbf{a}_1, \ldots, \mathbf{a}_n$ of M, the point group H_{SR} is represented by a set of integral matrices:

$$T\mathbf{a}_i = \sum_{j=1}^{n} \mathbf{a}_j \Gamma_{ji}(T), \qquad T \in H_{SR}. \tag{6.1}$$

After embedding M on an n-dimensional lattice Σ generated by the basis $\mathbf{a}_{1s}, \ldots, \mathbf{a}_{sn}$ and through the correspondence

$$\mathbf{a}_i \to \mathbf{a}_{is} = (\mathbf{a}_i, \mathbf{a}_{Ii}), \qquad i = 1, \ldots, n, \tag{6.2}$$

the elements T become a point-group transformation for Σ in terms of the same set of matrices:

$$T\mathbf{a}_{is} = \sum_{j=1}^{n} \mathbf{a}_{js} \Gamma_{ji}(T), \qquad T \in H_{SR}. \tag{6.3}$$

In order to be able to say that the lattice Σ is left invariant by T, the concept of a metric is needed [otherwise one could say that the whole group $Gl(n, \mathbb{Z})$ leaves Σ invariant]. As we have seen, there is no unique metric in the superspace which is left invariant by H_{SR} and if one continued in that direction one would arrive at the concept of multimetrical space, as briefly discussed in the previous section.

Here, we do not want to develop that approach further and in what follows we consider the superspace as being an affine space V_s only and we define the holohedry of the lattice Σ as being that of the homotheties of the vector module M one gets from the orthogonal projection of Σ in the external space.

A point group K is then a subgroup of H_{SR} and is called a scale-rotation point group.

A scale-space group G is a subgroup of the affine group $A(n)$, an extension of the lattice translation group $U(n)$ by the point group K.

When referred to a basis of the lattice, the group G is faithfully represented, as usual, by a set of matrices. In the Seitz notation we write for the elements of G:

$$g = \{T|t\} \to A(g) = \{\Gamma(T)|(t_1, \ldots, t_n)\}. \tag{6.4}$$

A scale-space group generates in V_s a set of equivalent points having lattice periodicity. By strip-projection, one then obtains in physical space a set of equivalent points for the quasicrystal structure. Inflation/deflation for the equivalent quasicrystal points is only verified if appropriate conditions are imposed on the strip defining the occupied positions among those possible. Different strips can occur for different sets of equivalent positions.

Conversely, consider a set of points in space defining the quasicrystal structure and thus a vector module M and a scale-rotation holohedry H_{SR}. The embedding of M on Σ yields a lattice periodic pattern in superspace. Its symmetry, consisting of all affine transformations leaving the pattern invariant and satisfying the additional requirement of having:
as **pure translations**: the elements of the lattice translation group $U(n)$ of Σ;
as **homogeneous components**: the elements of a point group $K \subset H_{SR}$;
is then a scale-space group.

It is because of the lack of metrical conditions that the admitted transformations have been restricted in order to ensure a structural interpretation of these symmetry elements.

Instead of developing further the theory of scale-space groups, let us consider an example compatible with the one-dimensional octagonal tiling with vector module $M^0 = M$ [as in (3.1)] embedded in a scaling-invariant lattice Λ_2. The rotational holohedry of M is $H_R = \bar{1}$, because it is one dimensional. The scaling holohedry is $H_S = \check{2} = \{N_2\}$ and this results in the infinite cyclic group generated by $S = N_2$ as defined in (3.5) and (4.3). (In fact, that is not fully true because mirrors have been disregarded but that is not essential here.) So, the holohedral point group of M is

$$H_{SR} = \bar{1}\check{2} = \{\bar{1}, N_2\} \tag{6.5}$$

and we consider the symmorphic scale-space group $G = \Lambda_2 \bar{1}\check{2}$ having lattice Λ_2 and point group $K = \bar{1}\check{2}$.

In order to characterize in terms of Wyckoff positions the set of equivalent points representing atomic arrangements, only positions of finite multiplicity have to be considered (only those having a relatively low multiplicity are structurally relevant). Such positions are characterized by the fact that they have at least a site symmetry N_2^k, for some integral value k.

As already mentioned in § 4, the set of points with site symmetry N_ν^k forms a lattice $\Lambda_{\nu,k}$ having Λ_ν as sublattice. One can show that the index of Λ_ν in $\Lambda_{\nu,k}$

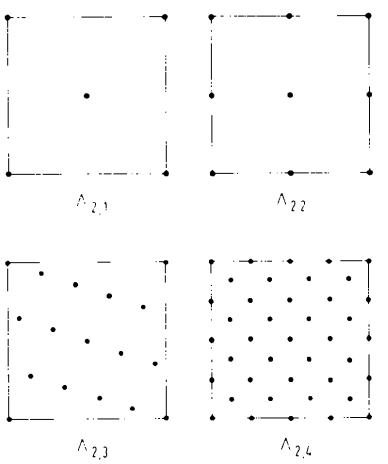


Fig. 17. Lattices $\Lambda_{2,k}$ consisting of the points having site symmetry $N_2^k = \check{2}^k$ in the frame where Λ_2 appears as a square lattice.

Table 1. *Equivalent positions in* $G_{SR} = \Lambda_2\bar{1}\check{2}$

Multiplicity	Wyckoff letter	site symmetry	Coordinates								
1	1(*a*)	$\bar{1}$	0, 0								
1	1(*b*)	$\bar{1}$	$\frac{1}{2}, \frac{1}{2}$								
2	2(*a*)	$\bar{1}\check{2}^2$	$\frac{1}{2}, 0$	$0, \frac{1}{2}$							
6	3(*a*)	$\check{2}^3$	$\frac{1}{7}, \frac{2}{7}$	$\frac{4}{7}, \frac{1}{7}$	$\frac{2}{7}, \frac{4}{7}$	$\frac{5}{7}, \frac{3}{7}$	$\frac{6}{7}, \frac{5}{7}$	$\frac{3}{7}, \frac{6}{7}$			
6	3(*b*)	$\check{2}^3$	$\frac{5}{14}, \frac{3}{14}$	$\frac{13}{14}, \frac{5}{14}$	$\frac{3}{14}, \frac{13}{14}$	$\frac{11}{14}, \frac{1}{14}$	$\frac{9}{14}, \frac{11}{14}$	$\frac{1}{14}, \frac{9}{14}$			
4	4(*a*)	$\check{2}^4$	$\frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}$					
8	4(*b*)	$\check{2}^4$	$\frac{1}{4}, 0$	$\frac{1}{2}, \frac{1}{4}$	$\frac{1}{4}, \frac{1}{2}$	$0, \frac{1}{4}$	$\frac{3}{4}, 0$	$\frac{1}{2}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{2}$	$0, \frac{3}{4}$	
8	4(*c*)	$\check{2}^4$	$\frac{1}{8}, \frac{1}{8}$	$\frac{3}{8}, \frac{1}{8}$	$\frac{7}{8}, \frac{3}{8}$	$\frac{1}{8}, \frac{7}{8}$	$\frac{1}{8}, \frac{5}{8}$	$\frac{7}{8}, \frac{1}{8}$	$\frac{7}{8}, \frac{7}{8}$	$\frac{5}{8}, \frac{7}{8}$	
8	4(*d*)	$\check{2}^4$	$\frac{5}{8}, \frac{1}{8}$	$\frac{3}{8}, \frac{5}{8}$	$\frac{3}{8}, \frac{3}{8}$	$\frac{1}{8}, \frac{3}{8}$	$\frac{5}{8}, \frac{3}{8}$	$\frac{5}{8}, \frac{5}{8}$	$\frac{7}{8}, \frac{5}{8}$	$\frac{3}{8}, \frac{7}{8}$	

. . . . . .

is given by

$$\text{index}\,(\Lambda_\nu \subset \Lambda_{\nu,2k+1}) = |\Delta q_k(\nu)| \tag{6.6}$$

$$\text{index}\,(\Lambda_\nu \subset \Lambda_{\nu,2k}) = |\Delta q_k(\nu) - 2| \tag{6.7}$$

where

$$\Delta q_k(\nu) = q_{k+1}(\nu) + q_{k-1}(\nu), \tag{6.8}$$

with $q_k(\nu)$ a generalized Fibonacci number, the solution of the recurrency relation

$$q_{k+1}(\nu) = \nu q_k(\nu) + q_{k-1}(\nu) \tag{6.9}$$

with initial values $q_0(\nu) = 0$ and $q_1(\nu) = 1$. In particular, for $\nu = 2$ the index I_k of Λ_2 in $\Lambda_{2,k}$ is given by

k	1	2	3	4	5	...
I_k	2	4	14	32	82	...

In Fig. 17 the lattices $\Lambda_{2,k}$ for $k = 1, 2, 3, 4$ are represented in the framework obtained from Λ_2 in the 'rest frame' by Euclidization as in (5.6), with $\tanh\alpha = 2^{1/2} - 1$. One sees that only $\Lambda_{2,3}$ is not a square lattice, but it becomes so if one considers the alternative Euclidization by $\tanh\alpha = 7 - 5\times 2^{1/2}$. The coordinates of the points are given with respect to the square-lattice basis of Λ_2 as in the figure mentioned above. The matrix representing N_2 is then as in (5.9).

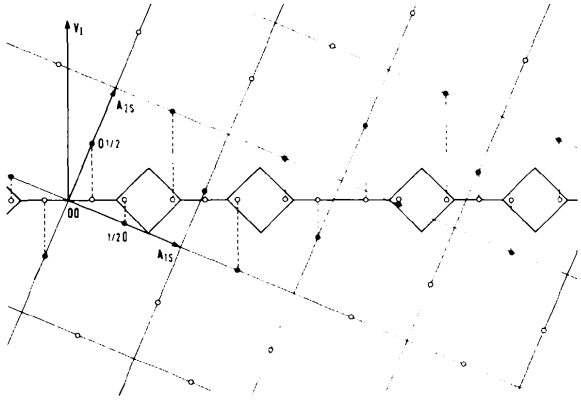


Fig. 18. Scaling invariant decoration of the one-dimensional octagonal tiling arising from points at the Wyckoff position 2(*a*) of the scale-space group $G = \Lambda_2\bar{1}\check{2}$ with fractional coordinates $0, \frac{1}{2}$ and $\frac{1}{2}, 0$ (see Table 1). Only the positions within a given strip region (the so-called occupied positions) result by projection on the physical space V in the points of the decoration. This decoration satisfies the same inflation-deflation rules as the tiling.

Using these results, one finds that the scale-space group $G = \Lambda_2\bar{1}\check{2}$ is generated by

$$G = \left\{(1,0), (0,1), \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 2 & 1 \\ 1 & 0 \end{pmatrix}\right\} \tag{6.10}$$

with $(1,0) = \mathbf{a}_{1s}$ and $(0,1) = \mathbf{a}_{2s}$ spanning a square lattice. Of course the latter property is not relevant here because we deal with an affine space.

The Wyckoff positions having low multiplicity are given in Table 1.

As already said, a set of equivalent points in the superspace only defines possible equivalent positions in space. It is the subset of the occupied positions which appears as set of equivalent points of the quasicrystal structure. In Fig. 18 it is shown how a 'decoration' of the one-dimensional octagonal tiling satisfying the same inflation-deflation rules as that tiling arises from the Wyckoff position 2(*a*) of a $\Lambda_2\bar{1}\check{2}$ invariant pattern within an appropriate strip region.

7. Concluding remarks

In this paper the starting point was a pattern observed by high-resolution electron microscopy of a quasicrystal in the octagonal phase and that pattern has been analyzed on the basis of a two-dimensional octagonal tiling. Step by step, new concepts have been introduced, showing how rich crystallography becomes once having passed 'through the looking glass' of plane reality. That reality is nevertheless essential because it is to obtain a better understanding of the complex crystallographic order observed in nature that the effort has been made.

It has been shown how it is possible to return from the superspace to the physical space, but the applicability of scale-space-group symmetry to existing structures has still not yet been demonstrated. Those who followed this exploration done in the spirit of Caroline MacGillavry will understand why it is not at all easy to give an answer to the question appearing as the title of this paper.

The partial support of the Stichting FOM of the Dutch National Science Foundation is gratefully acknowledged, as well as the stimulating views of my collegue T. Janssen.

APPENDIX
Glossary of some basic terms

Vector module M

It is defined in an m-dimensional space V (that of the quasicrystal) as the set of all integral linear combi-

nations of n basic vectors $\mathbf{a}_1, \ldots, \mathbf{a}_n$, where $n > m$, so that the basic vectors are linearly dependent on the reals. Usually, n is chosen in such a way that these vectors are linearly independent of the rationals. Consider for example in two dimensions ($m = 2$) a fivefold rotation R and an arbitrary vector $\mathbf{a}_1$. The vectors $\mathbf{a}_1$, $\mathbf{a}_2 = R\mathbf{a}_1$, $\mathbf{a}_3 = R^2\mathbf{a}_1$, $\mathbf{a}_4 = R^3\mathbf{a}_1$ are rationally independent, whereas if one adds $\mathbf{a}_5 = R^4\mathbf{a}_1$ they are not any more because $\sum_{i=1}^{5} \mathbf{a}_i = 0$. The set $\{\mathbf{a}_1, \ldots, \mathbf{a}_4\}$ forms a basis for M which is a vector module of rank 4 and dimension 2. It is sometimes convenient to consider $M' = \{\mathbf{a}_1, \ldots, \mathbf{a}_5\}$ and not M for reasons like those leading to the preference of a non-primitive lattice basis instead of a primitive one.

Superspace V_s

It is a higher-dimensional space having the same dimension n as the rank of M and containing the space V of the quasicrystal as a subspace.

Crystallographic lattice Σ

It is defined in V_s and is spanned by the basis $\mathbf{a}_{1s}, \ldots, \mathbf{a}_{ns}$ yielding by orthogonal projection on V the basis $\mathbf{a}_1, \ldots, \mathbf{a}_n$ of the vector module M. This projection is 1 to 1 if the vectors $\mathbf{a}_1, \ldots, \mathbf{a}_n$ are rationally independent. The lattice Σ describes the translational symmetry of the quasicrystal embedded in the superspace. Occupied atomic positions in space differing by vectors projected from the lattice Σ are considered to be 'translationally' equivalent.

Rotational point group K_R

The rotational point group K_R of the quasicrystal consists of m-dimensional rotations of finite order, which on the given basis of the vector module M define a group of invertible $n \times n$ matrices with integral entries. In V_s there exists for Σ a Euclidean metric tensor $(g_e)_{ik} = \mathbf{a}_{is} \cdot \mathbf{a}_{ks}$ left invariant by these transformations, which therefore are elements of an n-dimensional crystallographic point group representing the rotational point group of the embedded quasicrystal.

Superspace group G_0

It is the space-group symmetry of the quasicrystal embedded in the superspace. It has Σ as lattice symmetry and K_R as point group. We recall that only in the symmorphic case (where G_0 is the semi-direct product of the group of lattice translations with K_R) does the point group K_R leave the quasicrystal pattern invariant.

Scaling point group K_S

The scaling point group K_S of the quasicrystal consists of m-dimensional scaling transformations (*i.e.* discrete dilatations, possibly combined with rotations), which on the given basis of the vector module M become invertible integral $n \times n$ matrices of infinite order. Therefore, no invariant Euclidean metric in n dimensions exists for these transformations. In all the cases investigated so far, there exists, however, an indefinite metric tensor g_i for the lattice Σ expressible in terms of scalar products between lattice basis vectors $(g_i)_{hk} = \mathbf{a}_{hs} \circ \mathbf{a}_{ks}$ left invariant by the point group K_S. Accordingly, this group consists of crystallographic hyperbolic rotations leaving Σ invariant. With respect to the indefinite metric, the space V of the quasicrystal is such that these hyperbolic rotations leave V invariant and become scaling transformations once this subspace V is considered Euclidean.

Scale-space group G

It is the symmetry group of the quasicrystal which also includes scaling transformations. It has Σ as lattice of symmetry translations and a crystallographic point group K generated by K_R and K_S. The Euclidean subgroup of G is the n-dimensional space group G_0 considered above.

Automorph

A metric tensor g_{ik} defines on a lattice an integral binary quadratic form $Q = \sum_{i,k}^{n} g_{ik} x_i x_k$ in the coordinate variables $x_1, \ldots, x_n$ of the lattice points. A linear non-singular transformation A with integral entries: $x_i \to y_i = \sum_k^n A_{ik} x_k$ leads to an equivalent quadratic form Q'. If $Q = Q'$ the transformation A is said to be an automorph of the quadratic form. From a crystallographic point of view, a rotation leaving the lattice Σ invariant is an automorph of the quadratic form associated with the metric tensor g_e of the lattice. Point-group symmetries are thus automorphs of the integral binary quadratic form defined in terms of a basis of the lattice.

Negautomorph

Consider an invertible integral transformation N as A above but now such that $Q' = -Q$. Then N is a negautomorph of the quadratic form Q. Such point-group transformations are of importance in the case of an indefinite binary quadratic form (*i.e.* when the metric tensor is indefinite as the g_i considered above). As a simple example, consider in the plane two basis vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ with metric tensor defined by $\mathbf{a}_1 \circ \mathbf{a}_1 = 1$, $\mathbf{a}_2 \circ \mathbf{a}_2 = -1$ and $\mathbf{a}_1 \circ \mathbf{a}_2 = 0$. The vector $\mathbf{l} = \mathbf{a}_1 + \mathbf{a}_2$ has then length zero as $\mathbf{l} \circ \mathbf{l} = 0$. Such a vector is said to be isotropic. Consider

$$N = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

which is a mirror leaving $\mathbf{l}$ invariant. Then the quadratic form $Q = x_1^2 - x_2^2$ is transformed by N into

$Q' = x_2^2 - x_1^2 = -Q$. So N is a negautomorph of Q. In general, the product of two negautomorphs is an automorph.

Minkowski plane

Consider the two-dimensional space-time spanned by $\mathbf{a}_1$ and $\mathbf{a}_2$. Its points $\mathbf{x} = x_1\mathbf{a}_1 + x_2\mathbf{a}_2$ are called 'events' and have a space and a time coordinate (r, t). Multiplying the time coordinate by the speed of light c (normalized to 1), it also becomes a space coordinate. So we can put $x_1 = r$, $x_2 = ct = t$. Lorentz transformations L are linear transformations in the space-time leaving the light velocity invariant and thus also the value $x_1^2 - x_2^2$. A light wave propagates along events for which one has $x_1 = \pm x_2$. Accordingly, $\mathbf{a}_1 \pm \mathbf{a}_2$ are called light directions, where $\mathbf{a}_1$ is along the space axis and $\mathbf{a}_2$ along the time axis. Note that the metric tensor $g_{11} = \mathbf{a}_1 \circ \mathbf{a}_1 = 1$, $g_{22} = \mathbf{a}_2 \circ \mathbf{a}_2 = -1$, $g_{12} = \mathbf{a}_1 \circ \mathbf{a}_2 = 0$ is left invariant by the Lorentz transformation L which is therefore a hyperbolic rotation of the Minkowski plane. The scaling transformation induced by L along the light cone corresponds to the red shift (dilatation) or to the blue shift (contraction) of a light wave emitted from a moving source.

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Computation of Absorptive Form Factors for High-Energy Electron Diffraction

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(*Received* 30 *November* 1990; *accepted* 19 *April* 1991)

Abstract

An efficient procedure for calculating the contribution of the thermal diffuse scattering to the absorptive form factor is outlined. For an isotropic Einstein model all integrations could be performed analytically by using suitable functions to fit the elastic electron scattering amplitudes. The result is cast into a function subroutine which is available upon request. Computed values are compared with previous calculations and with measurements.

1. Introduction

The quantitative interpretation of electron diffraction patterns requires a comparison of the recorded patterns with calculations (Steeds, 1983). To perform a computation the Fourier coefficients of the lattice potential must be known. In a first approximation one considers only elastic scattering. In practice, however, inelastic processes scatter electrons out of the Bragg reflections into the background causing an attenuation of the reflections. The removal of electrons from the Bragg reflections can be described as an absorption. This absorption together with the increased background very severely affects the contrast in diffraction patterns, especially in the case of high-Z materials. The attenuation of the reflections can be incorporated into the dynamical theory by adding an imaginary part to the crystal potential (Yoshioka, 1957). The calculation of the diffuse back-

0108-7673/91/050590-08$03.00