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The Symmetry of Quasiperiodic Systems

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Abstract

A discussion is given of the symmetry groups of quasiperiodic systems. This is done in a formalism that uses space groups with dimension larger than three. Three main types are distinguished: modulated crystal phases, incommensurate composite structures and quasicrystals. For these the differences and similarities are discussed and the canonical embedding in higher-dimensional space is given, which requires some generalizations of earlier definitions. The equivalence relation between space groups for quasiperiodic systems is different from that for ordinary space groups, because of the presence of a distinct physical space. Apart from higher-dimensional space groups, some quasiperiodic systems have self-similarity properties. Examples are given and the relationship with space-group symmetry is discussed.

1. Introduction

In the past decades one has found an ever increasing number of structures with perfect order, but without lattice periodicity. These aperiodic 'crystals' are characterized by the fact that their diffraction spots are sharp and may be labelled by a finite number of indices, although this number may be larger than the dimension of the physical space. This means that the basis vectors are linearly dependent, but there is no linear combination with integer coefficients of their vectors which is zero, apart from the trivial case that all coefficients are zero. Such structures have been called quasiperiodic. Actually, lattice periodicity is a special case of quasiperiodicity. Then, the number of

integer indices is equal to the dimension of the space. Quasiperiodic systems are by no means rare (Janssen & Janner, 1987; Cummins, 1990). Among the minerals the common feldspar may have this property, many dielectrics, like quartz, show it in a certain temperature interval, and some years ago one had artificially made quasicrystals, which also belong to this category.

One can construct mathematical models of structures that are still more general, but nevertheless also perfectly ordered. For example, there are functions that are almost periodic (in the mathematical sense), but not quasiperiodic. (A quasiperiodic function is always almost periodic.) There are chains that can be constructed on a very simple deterministic algorithm, such as the Thue-Morse chain. Also, regular fractals, like the Sierpinski gasket, are perfectly ordered, but not quasiperiodic. All these systems touch on the border of crystallography and seek a generalization of crystallographic concepts. This can most easily be done for quasiperiodic systems to which we shall restrict our considerations here. Because they are in almost every respect similar to crystals, we shall call them aperiodic crystals, although, as the name indicates, generally they lack lattice periodicity.

Because there is no lattice periodicity the usual symmetry description for lattice periodic crystals breaks down. However, as we shall see, we can recover lattice periodicity because quasiperiodic systems are intersections of a lattice periodic system in a higher-dimensional space with a hyperplane that represents physical space. The symmetry description then comes down to the description of the higher-dimensional

system. Of course, one can stay in the physical space, but since there is a unique correspondence between the physical quasiperiodic system and the higher-dimensional one (the information content of both is the same) it is convenient to go to the unphysical higher-dimensional space, because there one can use traditional crystallographic concepts (de Wolff, 1974; Janner & Janssen, 1977; de Wolff, Janssen & Janner, 1981).

The important thing to do is to embed the physical system into an appropriate space. Since we can distinguish between different types of quasiperiodic systems, we can distinguish between different types of embedding as well. This point will be discussed in section two.

The symmetry group of the higher-dimensional system is a space group. One is then faced with the problem of when two such groups should be called the same. In three-dimensional space, two space groups are considered to be the same when they are isomorphic or, equivalently, when one can be transformed into the other by a change of reference frame, an affine transformation. This leads to 219 different space groups in three dimensions. If one allows only affine transformations that do not change the handedness of the frame, there are 230 space groups, with 11 enantiomorphic pairs. So the number of space groups is fixed by the equivalence relation and this in turn is dictated by the possibility of making physically a distinction between structures. It is not *a priori* clear what the equivalence relation should be for quasiperiodic systems. This problem is addressed in §3.

For certain classes of quasiperiodic systems there is an additional symmetry property, self-similarity. Scaling transformations play an important role in quasicrystals and in tilings, which are models for them. These transformations are directly related to the space-group symmetry, as will be shown in §4.

Some of the problems have been discussed before (de Wolff, 1974; Janner & Janssen, 1977; de Wolff *et al.*, 1981; Janner & Janssen, 1980). Here, we want to discuss a tentative unifying picture which generalizes earlier techniques. To make the paper self-consistent we shall briefly repeat some of the earlier work.

2. Embedding of quasiperiodic systems

2.1. Modulated crystal phase

The diffraction pattern of a quasiperiodic system consists of sharp Bragg peaks at positions that can be labelled by a finite number of integers h_1, \dots, h_n . This means that a diffraction vector can be written as

$$\mathbf{k} = \sum_{i=1}^n h_i \mathbf{a}_i^*, \quad h_i \text{ integer}, \quad (2.1)$$

where $\mathbf{a}_1^*, \dots, \mathbf{a}_n^*$ are basis vectors. The collection of

vectors (2.1) is in principle a dense set; there is no minimum distance. However, in practice the set is discrete. This means that observed peaks with an intensity above a certain threshold are discrete. This is because the intensities go to zero for high values of the indices.

If one describes the system with a density function $\rho(\mathbf{r})$, its Fourier decomposition looks like

$$\rho(\mathbf{r}) = \sum_{\mathbf{k} \in M^*} \hat{\rho}(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{r}). \quad (2.2)$$

The set of vectors M^* consists of all vectors of the form (2.1). It is called the Fourier module of $\rho(\mathbf{r})$. The number n of basis vectors is the rank of the module and its dimension d is the dimension of the physical space, usually three, but sometimes two or one.

Such a quasiperiodic function can be obtained from a function on an n -dimensional torus. Suppose f is a function of n variables and is periodic in each of them:

$$\begin{aligned} f(x_1, \dots, x_n) &= f(x_1 + 1, x_2, \dots, x_n) = \dots \\ &= f(x_1, \dots, x_{n-1}, x_n + 1). \end{aligned}$$

For n mutually irrational numbers $\alpha_1, \dots, \alpha_n$ we can define a function $g(x)$ by

$$g(x) = f(\alpha_1 x, \dots, \alpha_n x). \quad (2.3)$$

The Fourier components of $g(x)$ then belong to wave numbers $k = 2\pi(h_1/\alpha_1 + \dots + h_n/\alpha_n)$, where h_1, \dots, h_n are integers. In other words, the Fourier module of the quasiperiodic function $g(x)$ has rank n and dimension one. One can show that every quasiperiodic function is the restriction of a periodic function in a number of variables that is equal to the rank of the Fourier module. The problem is how to construct this periodic function.

A typical case is that of a displacively modulated crystal. The atoms of an ordinary crystal with space-group symmetry are displaced in such a way that the displacement itself is (quasi-) periodic. If the periodicity of the latter is irrational with respect to the periodicity of the starting crystal, which is called the basic structure, the modulated crystal is no longer periodic, but it is quasiperiodic. If the atoms of the basic structure have positions $\mathbf{n} + \mathbf{r}_j$, where \mathbf{n} is a lattice vector and \mathbf{r}_j the position of the j th atom inside the unit cell of Λ ($j = 1, \dots, s$, with s the number of atoms in the unit cell), the positions of the atoms in the modulated crystal are

$$\begin{aligned} \mathbf{r}(\mathbf{n}_j) &= \mathbf{n} + \mathbf{r}_j + \mathbf{u}_j(\mathbf{n}) \\ &= \mathbf{n} + \mathbf{r}_j + \sum_{\mathbf{q} \in \Pi^*} \hat{\mathbf{u}}_j(\mathbf{q}) \exp(i\mathbf{q} \cdot \mathbf{n}). \end{aligned} \quad (2.4)$$

The displacement field $\mathbf{u}_j(\mathbf{n})$ has Fourier module Π^* . If $(\mathbf{a}_1^*, \mathbf{a}_2^*, \dots, \mathbf{a}_d^*)$ is a basis for the reciprocal lattice Λ^* and $(\mathbf{a}_{d+1}^*, \dots, \mathbf{a}_n^*)$ one for Π^* , the Fourier

module M^* of the modulated system has basis $(\mathbf{a}_1^*, \dots, \mathbf{a}_n^*)$. In the diffraction pattern the spots may be labelled with n integers.

Associated with the quasiperiodic modulated phase is a periodic structure, called the average structure. It is obtained from the modulated crystal by bringing each atom (2.4) back to a unit cell of Λ . So the lattice coordinates of the points in the unit cell are

$$x_i(\mathbf{n}_j) = \text{frac} [\mathbf{a}_i^* \cdot \mathbf{r}_j + \mathbf{a}_i^* \cdot \mathbf{u}_j(\mathbf{n})], \quad i = 1, \dots, d. \quad (2.5)$$

A simple example of a modulated crystal is given by

$$\mathbf{r}(\mathbf{n}_j) = \mathbf{n} + \mathbf{r}_j + \mathbf{A}_j \sin(\mathbf{q} \cdot \mathbf{n} + \Phi_j), \quad j = 1, \dots, s. \quad (2.6)$$

Then $\mathbf{a}_i^* = \mathbf{q}$ and $n = 4$, if the coordinates of \mathbf{q} in the reciprocal-lattice basis are not all rational.

Besides the displacive modulation, one may also have an occupation modulation: a (possibly displaced) site may be occupied by atomic species A or B , with probability p and $1 - p$, respectively. Or one of two sites may be occupied by an atom with probabilities p and $1 - p$. If this probability is a periodic function of position, the system is quasiperiodic. Suppose the probability of finding atom A in the position $\mathbf{n} + \mathbf{r}_j$ is given by $p_j(\mathbf{q} \cdot \mathbf{n})$, where p_j satisfies $p_j(x) = p_j(x + 1)$, and the probability for an atom B being there by $1 - p_j(\mathbf{q} \cdot \mathbf{n})$. Then \mathbf{q} belongs to the Fourier module of the modulated system.

As stated before, a quasiperiodic structure may be embedded into a space with dimension equal to the rank of the Fourier module. The embedding is fixed as soon as the higher-dimensional lattice Σ is known. A basis for the reciprocal lattice Σ^* is $(\mathbf{a}_{s1}^*, \dots, \mathbf{a}_{sn}^*)$. For each atom in the quasiperiodic d -dimensional structure, there is a corresponding point in the unit cell of Σ . If the higher-dimensional space V_s is the direct sum of the physical space V_E and the additional space V_I , a point in V_E corresponding to an atom may be denoted by $(\mathbf{r}, 0)$, which has with respect to Σ lattice coordinates $x_{si} = \mathbf{a}_{si}^* \cdot (\mathbf{r}, 0)$. So the information on the whole (infinite) quasiperiodic system is mapped into the unit cell of Σ .

To find Σ and the meaning of the scalar product in V_s one considers the symmetry group K of the diffraction pattern, which is a d -dimensional point group. For every element R of K one can write its action on the basis vectors of M^* .

$$R\mathbf{a}_i^* = \sum_{k=1}^n \Gamma^*(R)_{ki} \mathbf{a}_k^*, \quad i = 1, \dots, n. \quad (2.7)$$

It is easily checked that the group of integer matrices $\Gamma^*(K)$ is a representation of K . As an integer representation it is not necessarily reducible, but, because K is finite, it is reducible as real representation. Indeed, the physical space V_E is left invariant by K .

So one can write

$$\Gamma^*(K) = D_E^*(K) \oplus D_I^*(K), \quad (2.8)$$

where the representations $D_E^*(K)$ and $D_I^*(K)$ themselves may also be reducible. Moreover, because K is finite, both of them are equivalent to orthogonal representations, K_E and K_I , respectively. So there is a positive definite metric in both V_E (the usual one, K_E being identical to K) and V_I . For the scalar product of $(\mathbf{r}_E, \mathbf{r}_I)$ and $(\mathbf{s}_E, \mathbf{s}_I)$ one can then take $\mathbf{r}_E \cdot \mathbf{s}_E + \mathbf{r}_I \cdot \mathbf{s}_I$, which gives a positive definite metric in V_s .

The basis for the n -dimensional representation $\Gamma^*(K)$ then can be chosen to be $\{(\mathbf{a}_k^*, \mathbf{b}_k^*), k = 1, \dots, n\}$. The j th basis vector has as component in V_E the j th basis vector \mathbf{a}_j^* of M^* . So the Fourier module M^* is just the projection of the lattice Σ^* in V_s , which is spanned by the basis of the representation $\Gamma^*(K)$. The reciprocal lattice Σ^* has a direct lattice Σ that is spanned by $\{(\mathbf{a}_k, \mathbf{b}_k), k = 1, \dots, n\}$ which satisfies $\mathbf{a}_k \cdot \mathbf{a}_l^* + \mathbf{b}_k \cdot \mathbf{b}_l^* = \delta_{kl}$. The action of K on the basis of Σ is given by the representation $\Gamma(K)$ with

$$\Gamma(R) = \text{transpose} [\Gamma^*(R^{-1})]. \quad (2.9)$$

For a modulated crystal one may distinguish between main reflections, which correspond to the reciprocal lattice of the average structure, and satellites. This implies that K does not mix $\mathbf{a}_1^*, \dots, \mathbf{a}_d^*$ and $\mathbf{a}_{d+1}^*, \dots, \mathbf{a}_n^*$. This means that the matrices $\Gamma(R)$ have the form

$$\Gamma(R) = \begin{pmatrix} \Gamma_E(R) & 0 \\ \Gamma_M(R) & \Gamma_I(R) \end{pmatrix}, \quad (2.10)$$

where $\Gamma_E(K)$ and $\Gamma_I(K)$ are, respectively, d - and $(n - d)$ -dimensional integral representations. The representation $\Gamma_E(K)$ is equivalent to the orthogonal representation K_E . It is, therefore, just a crystallographic point group. Its representation space is V_E and consequently one has $\mathbf{b}_j = 0$ for $j = 1, \dots, d$.

Now the lattices Σ and Σ^* are known and one can embed the quasiperiodic structure into V_s . One method follows from the observation that the projection from Σ^* to M^* is one to one. So for a vector \mathbf{q} in (2.4), which is a linear integer combination of $\mathbf{a}_{d+1}^*, \dots, \mathbf{a}_n^*$, the internal part \mathbf{q}_I is the same combination of $\mathbf{b}_{d+1}^*, \dots, \mathbf{b}_n^*$. One may now construct a periodic array of $(n - d)$ -dimensional hypersurfaces in V_s as

$$\left[\mathbf{n} + \mathbf{r}_j + \sum_{\mathbf{q} \in \Pi^*} \hat{\mathbf{u}}_j(\mathbf{q}) \exp(i\mathbf{q} \cdot \mathbf{n} + i\mathbf{q}_I \cdot \mathbf{t}), \mathbf{t} \right], \quad j = 1, \dots, s; \quad \mathbf{n} \in \Lambda; \quad \mathbf{t} \in V_I. \quad (2.11)$$

This set is invariant under lattice translations from Σ . The surfaces are called atomic surfaces. They are here unbounded, transverse (each intersects V_E) and in one-to-one correspondence with the $(n - d)$ -dimensional space V_I .

The other, more general, method, which is also applicable when one has a charge distribution instead of point atoms, starts from (2.2). Because \mathbf{k} from the Fourier module M^* is the unique projection of \mathbf{k}_s in Σ^* , a density function in the n -dimensional space is defined by

$$\rho(\mathbf{r}, \mathbf{t}) = \sum_{\mathbf{k} \in M^*} \hat{\rho}(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{r} + i\mathbf{k}_I \cdot \mathbf{t}). \quad (2.12)$$

It is easily shown that this function is left invariant by the lattice Σ and, therefore, has n -dimensional space-group symmetry.

Because the main reflections are mapped on main reflections by K , the latter is an ordinary d -dimensional crystallographic point group. Furthermore, if a structure can be seen as modulated, the displacements $\mathbf{u}_j(\mathbf{n})$ should be bounded. This means that on the average the atomic surfaces are parallel to V_I . This implies that there cannot be so-called mixing symmetries which do not leave V_E invariant.

2.2. Composite systems

A composite structure is one consisting of a finite number (larger than one) of subsystems, each subsystem being a (possibly modulated) crystal with lattice periodic (average) structure. We denote the lattice for subsystem μ by Λ_μ and its reciprocal lattice by Λ_μ^* . Suppose that $\{\mathbf{a}_i^{\mu*}\}$ forms a basis for Λ_μ^* . The total structure is quasiperiodic and not periodic if the Λ_i^* lattices are mutually incommensurate. The Fourier module is spanned by $\{\mathbf{a}_i^{\mu*}\}$ and, in addition, by eventual other modulation vectors. It is possible to give a description of such a modulated composite structure, but for the sake of simplicity we shall here suppose that modulation of a subsystem only occurs with the periodicity of another subsystem. Then the Fourier module is generated by $\{\mathbf{a}_i^{\mu*}\}$. Because the number of subsystems is finite the rank n is finite. Suppose $\{\mathbf{a}_i^*\}$ is a basis for M^* . Then one can express each $\mathbf{a}_i^{\mu*}$ in terms of the basis vectors, with integral coefficients (Janner & Janssen, 1980)

$$\mathbf{a}_i^{\mu*} = \sum_{k=1}^n Z_{ik}^{\mu} \mathbf{a}_k^*. \quad (2.13)$$

The embedding of the quasiperiodic structure follows from the construction of the lattice Σ which can be found in the same way as in the preceding section. The difference from a modulated crystal phase is that here none of the subsystems plays, *a priori*, a special role. Therefore, $\mathbf{b}_1^*, \dots, \mathbf{b}_d^*$ are not necessarily zero. Hence there are possibly n vectors \mathbf{b}_k^* in the $(n-d)$ -dimensional space V_I .

The positions of the atoms in subsystem μ can be written as

$$\mathbf{r}(\mathbf{n}j\mu) = \mathbf{r}_\mu^0 + \mathbf{n}_\mu + \mathbf{r}_{\mu j}, \quad (2.14)$$

where \mathbf{r}_μ^0 is the origin of Λ_μ , \mathbf{n}_μ a lattice vector from Λ_μ and $\mathbf{r}_{\mu j}$ inside the unit cell of the μ th lattice.

A first method to determine the embedding in V_s uses a mapping π_μ from V_I to V_E defined by

$$\pi_\mu \mathbf{r}_I = \sum_{ik} Z_{ik}^{\mu} (\mathbf{b}_k^* \cdot \mathbf{r}_I) \mathbf{a}_i^{\mu*}. \quad (2.15)$$

One defines a set of $(n-d)$ -dimensional hyperplanes by

$$(\mathbf{r}_\mu^0 + \mathbf{n}_\mu + \mathbf{r}_{\mu j} - \pi_\mu \mathbf{t}, \mathbf{t}), \quad \mathbf{t} \in V_I. \quad (2.16)$$

Its intersection with V_E (for $\mathbf{t} = 0$) is clearly the composite structure (2.14). To see that it is invariant under Σ , one takes $\mathbf{a}_i^{\mu*}$ which is, according to (2.13), the projection of $\mathbf{k}_s = \sum_k Z_{ik}^{\mu} (\mathbf{a}_k^*, \mathbf{b}_k^*) \in \Sigma^*$. Suppose $(\mathbf{a}_m, \mathbf{b}_m)$ is a basis vector of Σ . If one applies it to the set (2.16) one obtains

$$(\mathbf{r}_\mu^0 + \mathbf{n}_\mu + \mathbf{r}_{\mu j} - \pi_\mu \mathbf{t} + \pi_\mu \mathbf{b}_m + \mathbf{a}_m, \mathbf{t}). \quad (2.17)$$

The translation $\pi_\mu \mathbf{b}_m + \mathbf{a}_m$ belongs to Λ_μ , as one sees from its scalar product with $\mathbf{a}_i^{\mu*}$:

$$\begin{aligned} \mathbf{a}_i^{\mu*} \cdot (\pi_\mu \mathbf{b}_m + \mathbf{a}_m) &= \mathbf{a}_i^{\mu*} \cdot \mathbf{a}_m + \sum_I Z_{iI}^{\mu} (\mathbf{b}_I^* \cdot \mathbf{b}_m) \\ &= \left(\mathbf{a}_i^{\mu*}, \sum_I Z_{iI}^{\mu} \mathbf{b}_I^* \right) \cdot (\mathbf{a}_m, \mathbf{b}_m) \\ &= \mathbf{k}_s \cdot (\mathbf{a}_m, \mathbf{b}_m) \equiv 0 \pmod{2\pi}. \end{aligned} \quad (2.18)$$

This implies what one wants to prove. Hence, (2.16) is invariant under Σ and, therefore, the embedding of (2.14) for this Σ . This embedding is a generalization of that in Janner & Janssen (1980), where it is assumed that there is a host lattice for which one may choose d basis vectors with $\mathbf{b}_k^* = 0$.

One can find the embedding also by determining the coordinates of (2.14) with respect to Σ . The lattice coordinates of the points

$$(\mathbf{r}_\mu^0 + \mathbf{n}_\mu + \mathbf{r}_{\mu j}, 0) \quad (2.19)$$

with respect to $\{(\mathbf{a}_i, \mathbf{b}_i)\}$ are given by

$$c_i = \mathbf{a}_i^* \cdot (\mathbf{r}_\mu^0 + \mathbf{n}_\mu + \mathbf{r}_{\mu j}) = c_i^0 + x_i, \quad (2.20)$$

with $x_i = \text{frac}[\mathbf{n}_\mu \cdot \mathbf{a}_i^*]$. Because of the irrationality the points $\sum_i x_i (\mathbf{a}_i, \mathbf{b}_i)$ are not isolated, but dense in hyperplanes. These planes are the atomic surfaces. By construction, the set of atomic surfaces has periodicity Σ and the structure (2.14) as intersection with V_E .

A point $(\mathbf{r}, 0)$ has lattice coordinates $x_k = \mathbf{r} \cdot \mathbf{a}_k^*$ with respect to Σ and $x_i^{\mu} = \mathbf{r} \cdot \mathbf{a}_i^{\mu*}$ with respect to Λ_μ . Because of (2.13) one has the relation

$$x_i^{\mu} = \sum_{k=1}^n Z_{ik}^{\mu} x_k. \quad (2.21)$$

On the other hand, the coordinates x_k are not completely determined by x_i^{μ} , because Z^{μ} does not have an inverse, but only a pseudo-inverse (Mackay, 1977). If one diagonalizes Z^{μ} by left multiplication by an

integer $d \times d$ matrix P and right multiplication by an integer $n \times n$ matrix Q one has

$$(PZ^\mu Q)_{ij} = m_i \delta_{ij}. \quad (2.22)$$

Define the diagonal matrix D with diagonal elements m_i^{-1} . Then the pseudo-inverse

$$\bar{Z}^\mu = Q \text{ transpose } (D)P \quad (2.23)$$

satisfies $Z^\mu \bar{Z}^\mu Z^\mu = Z^\mu$, $\bar{Z}^\mu Z^\mu \bar{Z}^\mu = \bar{Z}^\mu$ and $Z^\mu \bar{Z}^\mu =$ identity in d dimensions.

The quantity x_k can be written as

$$x_k = \sum_{j=1}^d \bar{Z}_{kj}^\mu x_j^\mu + v_k, \quad k = 1, \dots, n. \quad (2.24)$$

These equations can be solved from

$$\begin{aligned} \sum_k Z_{ik}^\mu x_k &= \sum_{kj} Z_{ik}^\mu \bar{Z}_{kj}^\mu x_j^\mu + \sum_k Z_{ik}^\mu v_k \\ &= x_i^\mu + \sum_k Z_{ik}^\mu v_k. \end{aligned} \quad (2.25)$$

Hence x_k is only determined up to v_k in the null space of Z^μ . However, if v_k is in the null space, the line $\lambda \sum_k v_k (\mathbf{a}_k, \mathbf{b}_k)$ with $\lambda \in \mathbb{R}$ belongs to $(-\pi_\mu \mathbf{t}, \mathbf{t})$ because for $\mathbf{s} = \lambda \sum_k v_k \mathbf{b}_k$ one has

$$\lambda \sum_k v_k \mathbf{a}_k + \pi_\mu \left(\lambda \sum_k v_k \mathbf{b}_k \right) = 0. \quad (2.26)$$

Therefore, the null space of Z^μ corresponds exactly to the atomic surface for subsystem μ .

The atomic surfaces are no longer flat if one takes modulation into account. In (2.14) one has to add a displacement term. If its Fourier module belongs to M^* there is a displacement function for each μ , which may be embedded, giving a displacement for each μ and for each value of \mathbf{r}_I . Moreover, the displacement has translation symmetry Σ .

The fact that, generally, one cannot distinguish main reflections means that composite structures may have, in principle, point-group symmetry that is not a d -dimensional crystallographic one, or a mixing point group. We shall discuss two simple examples.

Consider a three-dimensional composite structure with five subsystems. Suppose \mathbf{e}_m is a vector $(\cos 2\pi m/5, \sin 2\pi m/5, 0)$ ($m = 1, \dots, 5$) and $\mathbf{e}_6 = (0, 0, a)$. Consider five lattices Λ_μ^* spanned by \mathbf{e}_6/a^2 , \mathbf{e}_μ and $\mathbf{e}_{\mu+1}$ (or \mathbf{e}_1 if $\mu = 5$).

Furthermore, there is one atom per unit cell per subsystem and $\mathbf{r}_\mu^0 = \mu \mathbf{e}_6/5$. Then the Fourier module has rank 5. The system consists of layers with oblique symmetry, such that each layer is rotated over 72°

with respect to the one above. The matrices Z^μ are

$$\begin{aligned} Z^1 &= \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \\ Z^2 &= \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \dots, \\ Z^5 &= \begin{pmatrix} 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \end{aligned} \quad (2.27)$$

The symmetry group of M^* is $\bar{5}m$, which is not a three-dimensional crystallographic point. The atomic surfaces are two-dimensional hyperplanes. The symmetry of the embedded structure is a symmorphic 5D space group.

As an example of a mixing symmetry consider the following 2D composite structure with four subsystems. The basis and origins with respect to an orthonormal reference frame in the plane are given as follows. For $\mu = 1$ $\{(a, b), (0, 1); (0, 0)\}$, for $\mu = 2$ $\{(a, -b), (0, 1); (-a/2, 1 + b/2)\}$, for $\mu = 3$ $\{(c, -d), (0, 1); (c, \frac{1}{2} - d)\}$, and for $\mu = 4$ $\{(c, d), (0, 1); (c/2, \frac{1}{2} + d/2)\}$ with the relations $c = a/(1 + 2b)$, $d = b/(1 + 2b)$. The Fourier module is of rank 3. The bases for Λ_μ^* are $\{(1/a, 0) (-b/a, 1)\}$, $\{(1/a, 0), (b/a, 1)\}$, $\{(1/c, 0), (d/c, 1)\}$ and $\{(1/c, 0), (-d/c, 1)\}$ for $\mu = 1, 2, 3, 4$, respectively.

$$\begin{aligned} Z^1 &= \begin{pmatrix} 1 & -1 & 0 \\ 0 & -1 & 1 \end{pmatrix}, & Z^2 &= \begin{pmatrix} 1 & -1 & 0 \\ 0 & 1 & 1 \end{pmatrix}, \\ Z^3 &= \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix}, & Z^4 &= \begin{pmatrix} 1 & 1 & 0 \\ 0 & -1 & 1 \end{pmatrix}, \end{aligned} \quad (2.28)$$

when the basis of M^* is chosen to be

$$\mathbf{a}_1^* = ([1 + b]/a, 0), \quad \mathbf{a}_2^* = (b/a, 0), \quad \mathbf{a}_3^* = (0, 1). \quad (2.29)$$

These three vectors are projections of $(\mathbf{a}_k^*, \mathbf{b}_k^*)$ with

$$\mathbf{b}_1^* = -b/a, \quad \mathbf{b}_2^* = (1 + b)/a, \quad \mathbf{b}_3^* = 0. \quad (2.30)$$

Then the three vectors $(\mathbf{a}_k^*, \mathbf{b}_k^*)$ span a cubic lattice, the atomic lines are straight lines, determined by Z^μ . With respect to the cubic lattice they are

$$\begin{aligned} &(\lambda, \lambda, \lambda), \quad (0, \frac{1}{2}, \frac{1}{2}) + (\mu, \mu, -\mu), \\ &(\frac{1}{2}, \frac{1}{2}, 0) + (\nu, -\nu, \nu), \quad (\frac{1}{2}, 0, \frac{1}{2}) + (\rho, \rho, \rho), \end{aligned} \quad (2.31)$$

where λ, μ, ν, ρ are real numbers. This set of lines is invariant under the 3D space group $Pn\bar{3}$. This implies systematic extinctions as a consequence of the non-primitive translations, and intensity equalities of spots connected by the tetrahedral point group. This shows that in principle such hidden symmetries may be present. Notice that the point group of M^* is only

pm̄m̄. The standard embedding would give $b_1^* = p$, $b_2^* = q$, $b_3^* = 0$ and no cubic lattice would result. It is only from the observation of additional symmetry relations that one gets a clue to the higher symmetric lattice. Also the phasonless quasicrystals discussed by Levitov (1989) belong to this category.

2.3. Long-period out-of-phase boundary systems

Out-of-phase boundaries in alloys give another example of possibly quasiperiodic systems. A typical example is an alloy with approximate composition AB_3 with atoms on the sites of a f.c.c. lattice. If the composition is AB_3 three sites are taken by a *B* atom, one by an *A* atom. The result is simple cubic. This symmetry can be broken by out-of-phase boundaries. This is a collection of planes over which the site taken by the *A* atom changes. If the planes are periodically or quasiperiodically arranged the structure is quasiperiodic. It can be viewed as a displacive or as an occupation modulation (Planès, 1990).

Suppose that the atoms are situated at positions \mathbf{r}_j in the unit cell and that the out-of-phase boundaries form a family of parallel planes, with wave vector \mathbf{q} [perpendicular to the family, with length = (interplanar distance)⁻¹]. If one crosses a boundary the atoms are displaced by a vector \mathbf{a} such that $\mathbf{r}_j + \mathbf{a} = \mathbf{r}_j \pmod{\Lambda}$. In the conservative case ($\mathbf{q} \cdot \mathbf{a} = 0$) one can write the position of the atom originally at $\mathbf{n} + \mathbf{r}_j$ by $\mathbf{n} + \mathbf{r}_j + \mathbf{a}$ ent $[\mathbf{q} \cdot \mathbf{n}] = \mathbf{n} + \mathbf{r}_j + (\mathbf{q} \cdot \mathbf{n})\mathbf{a} - \text{frac}[\mathbf{q} \cdot \mathbf{n}]\mathbf{a}$. Because $\text{frac}[x]$ is a periodic function, this describes a displacively modulated crystal. Its basic lattice Λ is spanned by $\{\mathbf{a}_i \equiv \mathbf{a}_i + (\mathbf{q} \cdot \mathbf{a}_i)\mathbf{a}; i = 1, \dots, d\}$, the modulation function is $\text{frac}[x]$ and the wave vector \mathbf{q} . If the latter is incommensurate with respect to Λ^* , the structure is incommensurate. The embedding then is given by

$$(\mathbf{n} + \mathbf{r}_j + (\mathbf{q} \cdot \mathbf{n})\mathbf{a} - \text{frac}[\mathbf{q} \cdot \mathbf{n} + t], t). \quad (2.32)$$

The vectors of the Fourier module are

$$\mathbf{k} = \mathbf{H} - (\mathbf{H} \cdot \mathbf{a})\mathbf{q} + m\mathbf{q}, \quad \mathbf{H} \in \Lambda^*, \quad m \in \mathbb{Z}. \quad (2.33)$$

In the non-conservative case ($\mathbf{q} \cdot \mathbf{a} \neq 0$) the local composition changes near the out-of-phase boundaries. In that case it is more convenient to describe the structure as an occupation modulated structure. The site j is occupied with probability p_j by atom *A* and with probability $1 - p_j$ by an atom *B*. In the cubic structure $p_j = 1$ for one site and $p_k = 0$ for the three other sites. In the presence of out-of-phase boundaries the site $\mathbf{n}j$ is occupied with probability $p_j(\mathbf{q} \cdot \mathbf{n})$, where p_j is a periodic function with period N , depending on the number of boundaries one has to cross to come back to the same situation. The embedding consists of straight lines $(\mathbf{n} + \mathbf{r}_j, t)$ on which the probability function is periodic. This is not necessarily a step function.

As an example consider a f.c.c. lattice. Domains with *A* in (000) alternate with domains with *A* in $(0\frac{1}{2}\frac{1}{2})$. The three other sites are taken by *B*'s. So $N = 2$. The out-of-phase boundaries are supposed to have wave vector \mathbf{q} in the *x* direction. The structure factor is given by

$$F(\mathbf{H}) = \sum_{\mathbf{n}j} \{f_A p_j(\mathbf{q} \cdot \mathbf{n}) + f_B [1 - p_j(\mathbf{q} \cdot \mathbf{n})]\} \times \exp(2\pi i \mathbf{H} \cdot \mathbf{n}), \quad (2.34)$$

which has wave vectors belonging to the Fourier module $\{h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c} + m\mathbf{q}\}$. If $\mathbf{q} = \alpha\mathbf{a}^*$ the lattice Σ is generated by $(\mathbf{a}, -\alpha)$, $(\mathbf{b}, 0)$, $(\mathbf{c}, 0)$ and $(0, 1)$, with reciprocal lattice generated by $(\mathbf{a}^*, 0)$, $(\mathbf{b}^*, 0)$, $(\mathbf{c}^*, 0)$ and $(\mathbf{q}, 1)$. Because of the centring the Fourier module vectors satisfy $h + k = \text{even}$ and $h + l = \text{even}$. On the lines through $\mathbf{n} + \mathbf{r}_j$ parallel to V_j , the function $p_j(t)$ changes between 0 and 1 in a periodic way (Fig. 1).

2.4. Quasicrystals

In recent years, several phases of alloys have been reported with a diffraction pattern with a non-crystallographic point-group symmetry, such as a five- or eightfold axis. They have been called quasicrystals. Often these structures resemble decorated tilings, *i.e.* quasiperiodic space-filling patterns composed of volumes of a finite number of shapes. Each volume of a certain type contains a number of atoms in a fixed arrangement. So they can be considered as a kind of unit cell.

A generally accepted definition of quasicrystals is still missing. In earlier sections one has seen systems with non-crystallographic point-group symmetry which should be considered as composite structures. On the other hand, one can construct quasiperiodic

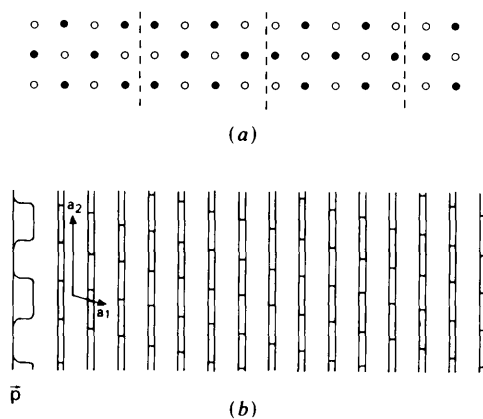


Fig. 1. Embedding of a system with incommensurate out-of-phase boundaries. (a) Distribution of atoms *A* and *B* over the sites 1 ($x + y = \text{even}$) and 2 ($x + y = \text{odd}$). (b) Periodic distribution function in n -dimensional space. On each line is indicated the probability p of having an atom *A* at site 1. At the left the shape of this function is sketched.

tilings with a crystallographic point-group symmetry. So this point seems to be not too important. Also the fact that they resemble tilings is not general. Nevertheless, we shall restrict ourselves here mainly to tilings.

Using the procedure from the preceding sections one can embed a quasicrystal starting from its diffraction pattern and determining the lattices Σ and Σ^* from the representation $\Gamma^*(K)$ of the point group. If one knows Σ it is straightforward to embed the structure into the higher-dimensional space. Here one inverts the procedure and starts from Σ . The periodic structure in V_s is obtained by attaching one or more atomic surfaces in each unit cell. For a tiling these atomic surfaces are parallel, otherwise the distance of the points would vary with the internal coordinate. For a modulated tiling bounded deviations from flatness are allowed. The atomic surfaces are not necessarily unbounded, like they were for modulated and composite structures. There is, however, a restriction to that. An atomic surface cannot end without the projection of the border on V_I coinciding with the border of an atomic surface nearby (in V_E) in projection. Otherwise atoms would disappear abruptly and eventually pop up at large distance, when the internal coordinate r_I changes.

One way is considering as atomic surface a copy of the projection of the unit cell of Σ on V_I . In each vertex of Σ such an atomic surface is attached. A well known example is the standard two-dimensional octagonal tiling. If $\mathbf{e}_m = [\cos(m\pi/4), \sin(m\pi/4)]$, the Fourier module is generated by $(\frac{1}{2}\mathbf{e}_0, \dots, \frac{1}{2}\mathbf{e}_3)$. The point group is $8mm$, the lattice Σ^* is generated by $\frac{1}{2}(\mathbf{e}_0, \mathbf{e}_0), \frac{1}{2}(\mathbf{e}_1, \mathbf{e}_3), \frac{1}{2}(\mathbf{e}_2, \mathbf{e}_2)$ and $\frac{1}{2}(\mathbf{e}_3, \mathbf{e}_1)$, and the lattice Σ by $(\mathbf{e}_0, \mathbf{e}_0), (\mathbf{e}_1, \mathbf{e}_3), (\mathbf{e}_2, -\mathbf{e}_2)$ and $(\mathbf{e}_3, \mathbf{e}_1)$. The projection of the unit cell is an octagon with diameter $(1+2^{1/2})$. If one puts such an octagon in each vertex of Σ , the intersection with every 2D plane parallel to V_E is formed by the vertices of a 2D octagonal tiling of the plane by squares and lozenges with an angle of 45° . The symmetry group of the 4D structure is the symmorphic space group $P8mm$. If one shifts the physical space V_E parallel to itself, the intersection point with the atomic surface in the origin moves over the octagon. When it reaches the border, the point in the origin vanishes, but another nearby point, which was not a vertex, now appears. For example, if the intersection point r_I with the physical space becomes $(\frac{1}{2} + \frac{1}{2}2^{1/2}, 0)$, the point in the origin of V_E 'jumps' to the point $(\frac{1}{2} - \frac{1}{2}2^{1/2}, 0)$.

Atomic surfaces may also be determined by the requirement that a vertex has a given minimal distance to other vertices. For the 2D dodecagonal lattice which has rank 4 the projection of the 4D Wigner-Seitz cell has a dodecagonal shape. The requirement that the minimal distance of vertices is $(2-3^{1/2})^{1/2}$ gives another dodecagon, which is rotated over 15° with respect to the first one. The first dodecagon

has a diameter of $1+2(1/3)^{1/2}$, the second one of $(2-3^{1/2})^{1/2}$.

It is not necessary either to put atomic surfaces in the vertices of Σ . If a point \mathbf{r}_E is present in V_E as soon as there are vertices $\mathbf{n}_{E1}, \dots, \mathbf{n}_{Ep}$ ($\mathbf{n}_1, \dots, \mathbf{n}_p \in \Sigma$), one has to attach a copy of the intersection of the projections of the atomic surfaces in $\mathbf{n}_1, \dots, \mathbf{n}_p$ on V_I to a point in V_s that has external component \mathbf{r}_E such that the projection coincides with the intersection of projections. To keep the same symmetry group one applies the space group to the atomic surface found. Its orbit gives a finite number of atomic surfaces in the unit cell of Σ .

As an example, consider the case that each square of the octagonal tiling has an atom exactly in the middle. An atomic surface Ω in $\mathbf{n} \in \Sigma$ gives a vertex if $(\mathbf{n}_E, 0)$ belongs to Ω . This is the corner of a square if the origin belongs to the intersection of $\Omega, \Omega + \mathbf{e}_0, \Omega + \mathbf{e}_2, \Omega + \mathbf{e}_0 + \mathbf{e}_2$ in one case, to that of $\Omega, \Omega + \mathbf{e}_1, \Omega + \mathbf{e}_3$ and $\Omega + \mathbf{e}_1 + \mathbf{e}_3$ in the other. These intersections are squares (Fig. 2a). If one attaches a square at $\mathbf{r}_E = \frac{1}{2}(\mathbf{e}_0 + \mathbf{e}_2)$ or $\mathbf{r}_E = \frac{1}{2}(\mathbf{e}_1 + \mathbf{e}_3)$, respectively, such that its projection coincides with these squares in V_I , these atomic surfaces produce the desired result. Analogously, if one wants to have an atom in the middle of each edge of the tiling, the intersection of two atomic surfaces shifted over \mathbf{e}_i ($i=1, \dots, 4$) is a hexagon (Fig. 2b), which is the shape of the desired atomic surface to be put in $(\frac{1}{2}000)$ and its orbit $(0\frac{1}{2}00), (00\frac{1}{2}0), (000\frac{1}{2})$. The full structure then still has $P8mm$ symmetry.

A tiling may also have a non-symmorphic space group. The construction for such a structure is quite similar to that of the example above. Consider as an example the non-symmorphic 4D space group with point group $8mm$. Its generators are $(x, y, z, t) \rightarrow (-t, x, y, z), (x, y, z, t) \rightarrow (t + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2})$ and the lattice Σ . The set of points $(0000), (\frac{1}{2}0\frac{1}{2}0), (0\frac{1}{2}0\frac{1}{2})$ and $(\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2})$ in the unit cell is left invariant. Together with Σ they generate, however, a new octagonal lattice with basis vectors $(0\frac{1}{2}0 - \frac{1}{2}), (\frac{1}{2}0\frac{1}{2}0), (0\frac{1}{2}0\frac{1}{2}), (-\frac{1}{2}0\frac{1}{2}0)$. Attachment of an octagon in each point with $\frac{1}{4}$ of the area of the projection of the unit cell of Σ would give again an octagonal tiling. If one deforms the octagons

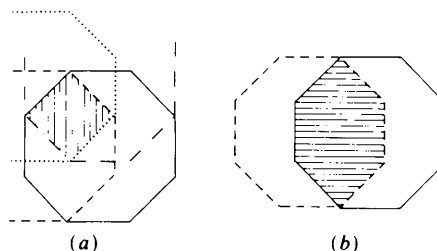


Fig. 2. (a) Overlap region in projection on V_I of four octagons at $0000, 1000, 0010$ and 1010 . The shape of the overlap is the shape of an atomic surface projection for an atom inside a square. (b) Atomic surface for an atom on an edge.

differently for the four atomic surfaces in the unit cell and in such a way that they are left invariant by the tetragonal subgroup, the translation symmetry is again Σ . Because one wants to keep the situation that the border of a projected surface is the projection of another one, the deformation is in the horizontal direction parallel to V_E . The atomic surfaces in $(\frac{1}{2}0\frac{1}{2}0)$ and $(0\frac{1}{2}0\frac{1}{2})$ have tetragonal site symmetry and can, for that reason, be divided into fundamental domains. Choosing a displacement (in the V_E direction) of one such domain of the surface at $(\frac{1}{2}0\frac{1}{2}0)$ the displacement of the other and those at $(0\frac{1}{2}0\frac{1}{2})$ follow from the space-group transformation. In Fig. 3 an example of such a displacement is given. For vanishing displacement ($\varepsilon = 0$) the symmetry group is a symmorphic space group with a translation group that has Σ as sublattice of index four. If $\varepsilon \neq 0$ the symmetry is broken. The symmetry group is a non-symmorphic subgroup of the former, its translation subgroup is exactly Σ . The corresponding tiling (Fig. 4) is a deformation of the standard octagonal tiling. Its symmetry group is non-symmorphic. In principle such a symmetry lowering could occur at a phase transition.

Finally, it can be noticed that the requirement that the border of an atomic surface has the same projection on V_I as that for another one, is no longer necessary if the quasiperiodic tiling is given by an occupation distribution with n -dimensional space-group symmetry. If two atomic surfaces that correspond to two V_E positions that cannot be occupied simultaneously have an overlap in projection on V_I , one region is occupied with probability p . If this

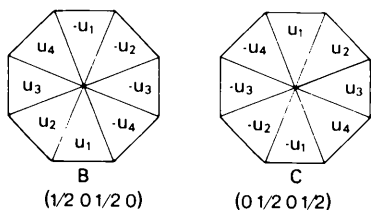


Fig. 3. Atomic surface for an octagonal tiling with non-symmorphic space group. In each fundamental domain its displacement is given: $u_i = \varepsilon e_i$, where e_i are the four basis vectors ($\cos m\pi/4$, $\sin m\pi/4$) ($m = 0, 1, 2, 3$).

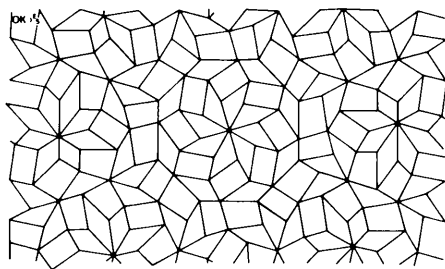


Fig. 4. The octagonal tiling resulting from the atomic surface of Fig. 3.

region is occupied, the other one is empty and *vice versa*.

2.5. Comparison of the structures

In the previous sections essentially three different types of quasiperiodic structures were discussed. Here we want to point out the differences and similarities. All these structures have sharp Bragg peaks that can be labelled with a number of integer indices that is larger than the dimension of the space. The characteristics become especially clear if one considers their embedding in a higher-dimensional space.

Examples of incommensurate modulated crystal phases are γ - Na_2CO_3 , several A_2BX_4 compounds, like K_2SeO_4 and Rb_2ZnCl_4 , in certain temperature intervals, and quartz in a tiny interval between the α and the β phase. The diffraction pattern consists of main reflections and satellites. Therefore, the point-group symmetry is crystallographic in physical space. The embedding into higher-dimensional space to get a periodic pattern consists of unbounded hypersurfaces which are in the average all parallel. This implies that mixing symmetries, which mix V_E and V_I , are not possible for these systems. The hypersurfaces may be straightened and an eventual occupation function defined on them changed to a constant in a continuous way. The result is then a lattice periodic system in V_E for which the Fourier module is a submodule of the quasiperiodic system.

Examples of composite structures are $\text{Hg}_{3-x}\text{AsF}_6$, $\text{TTF}_7\text{I}_{5-x}$ and intercalates. In these cases there is a host lattice, which gives a distinction between main reflections and satellites. In general, such a distinction is not possible. In that case also non-crystallographic point-group symmetry of the diffraction is possible. The embedding into higher-dimensional space consists of unbounded hypersurfaces, which are hyperplanes, eventually with a periodic modulation. The hyperplanes are not parallel. Therefore, mixed point-group symmetries are possible. Moreover, they are spanned by lattice vectors, i.e. they are in a rational direction in Σ . Therefore, they cannot be made parallel in a continuous way without changing the Fourier module. There is a one-to-one correspondence between the points of an atomic surface and V_I and, therefore, every path in V_I has a unique image in each atomic surface.

Examples of good quality quasicrystals are rather rare. One of the most ideal systems is AlCuFe . As model systems one has studied tilings of which the two- and three-dimensional Penrose tilings are the best known. Quasiperiodic tilings do not show a distinction between main reflections and satellites. Therefore, non-crystallographic point groups are possible. In fact, most of the systems studied have pentagonal, octagonal, dodecagonal, decagonal or icosahedral symmetry, but one can construct

quasiperiodic hexagonal tilings as well. The embedding into the higher-dimensional space consists of bounded atomic surfaces, which share a border with another one, when projected on V_I . The atomic surfaces are, on the average, parallel. Local absence of parallelism is due to modulation. Because of the parallelism they do not have mixing symmetries, although usually one lifts the Fourier module M^* to a hypercubic or other high-symmetry lattice.

Although the atomic surfaces are parallel, they can, generally, not be continuously changed to produce a periodic system. A path on V_I can be lifted to a path on atomic surfaces. One starts with a point P in V_I and considers an atomic surface for which the projection on V_I contains P . If one follows the path, the corresponding point moves over the atomic surface. Because Ω is bounded this point may arrive at the border. Because the projection of this border coincides with that of another atomic surface the lifted path may be continued on the latter (Fig. 5). This is equivalent to a motion over one atomic surface of which one identifies opposite parallel borders. The paths in V_I then give rise to paths on Ω . Two closed paths are called equivalent if they can be deformed into each other in a continuous way. The equivalence classes form a group which is characteristic for the topology. For a periodic system the atomic surfaces fit together in net planes. Because of the lattice periodicity the topology of the atomic surface is that of an $(n-d)$ -dimensional torus. So if the topology of the atomic surface is different from that of a torus, there is no possibility of changing the quasiperiodic structure in a continuous fashion into a periodic one. For a one-dimensional quasiperiodic structure of rank 2 (e.g. the Fibonacci chain), the atomic surfaces are line elements. Identification of the end points gives a circle. Therefore, such a system can continuously be deformed to a periodic system. The octagonal atomic surface for the $n=4, d=2$ octagonal tiling has the topology of a 2D surface of genus two, the dodecagonal atomic surface for the standard $n=4, d=2$ dodecagonal tiling is associated with a surface

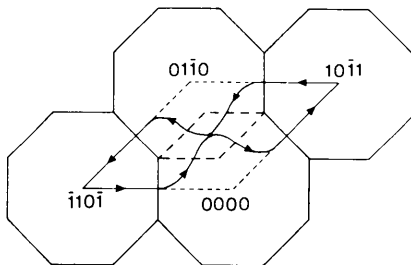


Fig. 5. Lift of a closed path in V_I to a path over atomic surfaces. When the point in V_I comes back for the first time its lifted point has shifted over $e_2 - e_3$. After two loops the lifted path closes. The latter cannot continuously be contracted to a point.

of genus three. The four pentagons for the $n=4, d=2$ Penrose tiling combine to two 2D surfaces of genus two. Therefore in these cases the quasiperiodic structures are certainly not modulated periodic structures.

The topology and the direction of the atomic surfaces, therefore, are of importance for the characterization of the different incommensurate and quasiperiodic structures. This has already been discussed by Frenkel, Henley & Siggia (1986) and by Kléman (1990). For internal dimension larger than two there is the problem that there is not a topological classification available.

3. Superspace groups

The embedded lattice periodic structures in n dimensions have as symmetry group an n -dimensional space group G . The structure of such a group is similar to that of an ordinary 3D space group. The lattice Σ spans the n -dimensional space V_S and is a normal subgroup of G . G itself is a discrete subgroup of the Euclidean group in n dimensions and the factor group G/Σ is isomorphic to the point group K , which is a subgroup of the n -dimensional orthogonal group. Mathematically speaking, G is an extension of K by $\Sigma \cong \mathbb{Z}^n$. If the extension is trivial, G is a symmorphic group, the semidirect product of \mathbb{Z}^n and K .

The abstract structure may be given using generators and relations. Suppose K is generated by R_1, \dots, R_p through q relations $\Phi_\mu(R_1, \dots, R_p) = 1$. The generators of Σ are the basis translations a_{si} ($i = 1, \dots, n$). For each $R \in K$ one chooses one element $r(R)$ in G which is mapped on R when taking the quotient G/Σ . Then G is generated by $\{a_{si}, r(R_j)\}$; $i = 1, \dots, n$; $j = 1, \dots, p$ through the relations

$$a_{si} + a_{sj} = a_{sj} + a_{si}, i, j = 1, \dots, n$$

$$R_j a_{si} = \sum_{k=1}^n \Gamma(R_j)_{ki} a_{sk}, i = 1, \dots, n; j = 1, \dots, p \quad (3.1)$$

$$\Phi_\mu[r(R_1), \dots, r(R_p)] = g_\mu \in \Sigma, \mu = 1, \dots, q.$$

Any group for which one can find generators satisfying these relations is isomorphic to G .

This is a compact but somewhat implicit specification of G . A more common one is writing the elements of G in the Wigner-Seitz notation as $\{R|v(R)\}$, where $R \in K$ and $v(R)$ a translation, not necessarily belonging to Σ . The most explicit way of giving the group is by specifying the action of $\{R|v(R)\}$ on a point with lattice coordinates x_i ($i = 1, \dots, n$) through

$$\{R|v(R)\} : (x_1, \dots, x_n) \rightarrow (x'_1, \dots, x'_n). \quad (3.2)$$

The translation part $v(R)$ can be decomposed into an intrinsic part and an origin-dependent part. The

former is given, when R^N is the unit element E , by

$$\mathbf{v}^i(R) = (1/N) \sum_{p=1}^N R^p \mathbf{v}(R) \equiv N_R \mathbf{v}(R) \pmod{\mathbb{Z}}. \quad (3.3)$$

It may occur that the intrinsic part of every $\mathbf{v}(R)$ vanishes, although the group is non-symmorphic. This is, for example, the case for the non-symmorphic $n=4$, $d=2$ group for the octagonal point group $8mm$. However, this is not special for the higher dimensions, In three dimensions it occurs, for example, for $I2_12_12_1$. It is the intrinsic part that is important for systematic extinctions. It is, usually, used in the notation for the space group.

In the case of modulated structures, the elements g of a space group G can be written as (g_E, g_I) , when g_E and g_I act in V_E and V_I , respectively. The elements g_E form a d -dimensional space group. It is, therefore, natural to use the symbols for these groups. One can use the fact that a basis for Σ^* can be chosen that has elements $\{(\mathbf{a}_i^*, 0), (\mathbf{a}_j^*, \mathbf{b}_j^*); i=1, \dots, d; j=d+1, \dots, n\}$. Because $\{\mathbf{a}_i^*\}$ is a basis for Λ^* one can decompose \mathbf{a}_{d+j}^* into reciprocal-lattice vectors:

$$\mathbf{a}_{d+j}^* = \sum_{k=1}^d \sigma_{jk} \mathbf{a}_k^*. \quad (3.4)$$

The basis of Σ is then given by

$$\begin{aligned} \mathbf{a}_{si} &= \left(\mathbf{a}_i, - \sum_{j=1}^{n-d} \sigma_{ji} \mathbf{b}_j \right) \quad (i=1, \dots, d); \\ \mathbf{a}_{sm} &= (0, \mathbf{b}_{m-d}) \quad (m=d+1, \dots, n), \end{aligned} \quad (3.5)$$

where $\mathbf{b}_i \cdot \mathbf{b}_j^* = \delta_{ij}$.

The matrix σ in (3.4) also has an invariant part σ^i defined by

$$\sigma^i = (1/|K|) \sum_{R \in K} \Gamma_I(R)^{-1} \sigma \Gamma_E(R), \quad (3.6)$$

which satisfies $\Gamma_I(R) \sigma^i = \sigma^i \Gamma_E(R)$ for every $R \in K$. Now consider a translation $\mathbf{v}(R)$. If the external part is $\mathbf{v}_E = \sum_i v_{\alpha} \mathbf{a}_i$ the internal part is

$$\begin{aligned} \mathbf{v}_I &= - \sum_{i=1}^d \sum_{j=1}^{n-d} \sigma_{ji} v_i \mathbf{b}_j + \sum_{j=1}^{n-d} v_{d+j} \mathbf{b}_j \\ &\equiv \tau(R) - \sum_{i=1}^d \sum_{j=1}^{n-d} \sigma_{ji}^i v_i \mathbf{b}_j. \end{aligned} \quad (3.7)$$

It is easily shown that $\tau(R)$ under a shift of origin $(\mathbf{r}_E, \mathbf{r}_I)$ changes by $(1-R_I)\mathbf{r}_I$. This means that

$$\tau^i = (1/N) \sum_{p=1}^N R_I^p \left(\mathbf{v}_I + \sum_{ji} \sigma_{ji}^i v_i \mathbf{b}_j \right), \quad (R^N = 1) \quad (3.8)$$

is invariant under a change of origin, and can be used to indicate the intrinsic internal part. Notice that this is different from the internal component of the translation $\mathbf{v}^i(R)$ which is just $(1/N) \sum_p R_I^p \mathbf{v}_I$.

When speaking of different space groups one usually means non-equivalent space groups. In ordinary crystallography two space groups are considered to be equivalent if there is an affine transformation $\{S|\mathbf{t}\}$, consisting of a linear transformation S with positive determinant and a translation \mathbf{t} which connects both groups: for each $\{R|\mathbf{v}\}$ in G there is an $\{R'|\mathbf{v}'\}$ in G' such that

$$\{R'|\mathbf{v}'\} = \{S|\mathbf{t}\} \{R|\mathbf{v}\} \{S|\mathbf{t}\}^{-1}. \quad (3.9)$$

This transformation describes a change of reference frame. The requirement $\det(S) > 0$ guarantees that the handedness is the same. With this definition one arrives at 230 space groups, belonging to 73 arithmetic, 32 geometric and 14 Bravais classes. For quasiperiodic systems one cannot simply take over this definition because it disregards the fact that V_E is a distinct subspace. The affine transformation should keep this distinction, but on the other hand different embeddings of the same structure in V_E should have equivalent space groups. Since the embedding is constructed starting from the diffraction pattern, two space groups for quasiperiodic systems are equivalent if they are connected by an affine transformation $\{S|\mathbf{t}\}$ such that the dual S^* leaves V_E invariant and has positive determinant for its restriction to V_E . One has to distinguish three types.

The first case is where one has a lattice of main reflections. The representation $\Gamma(K)$ may be chosen in the form (2.10). Then its dual leaves V_E invariant. The matrix groups K_E and K_I are subgroups of $O(d)$ and $O(n-d)$, respectively. Two point groups are geometrically equivalent if K_E is conjugated to K'_E and K_I to K'_I in their respective orthogonal groups. The matrix groups $\Gamma(K)$ and $\Gamma'(K)$ are arithmetically equivalent if $S\Gamma(K) = \Gamma'(K)S$ for some integral matrix S of the form

$$S = \begin{pmatrix} S_E & 0 \\ S_M & S_I \end{pmatrix}, \quad \det(S_E) = 1. \quad (3.10)$$

Two space groups with given $\Gamma(K)$ are equivalent if there is such an S which in addition does not change $\Gamma(K)$ and therefore is an element of the normalizer of $\Gamma(K)$ in $GL(n, \mathbb{Z})$ and which maps the translation parts of one group to those of the other, modulo a lattice translation and a shift of origin. In this way one finds 775 non-equivalent groups for modulated incommensurate systems with $d=3$ and $n=4$.

The second case is that of quasiperiodic crystals with a non-mixing point group, *i.e.* one which leaves V_E and V_I invariant. So the elements of K are pairs (R_E, R_I) . Also here $K \sim K'$ if and only if $K_E \sim K'_E$ and $K_I \sim K'_I$. To specify an arithmetic point group one has to give the group $\Gamma(K)$ and to specify the representation $D_I(K)$ contained in $\Gamma(K)$. If $\chi(K)$ is the character of this representation, the projection

operator of V_s to the representation space of D_I is

$$\pi_I = (1/|K|) \sum_{R \in K} \chi^*(R) \Gamma(R^{-1}). \quad (3.11)$$

Hence $\Gamma(K)$ and $\Gamma'(K)$ are arithmetically equivalent if there is an element $S \in GL(n, \mathbb{Z})$ such that $S\Gamma(R) = \Gamma'(R)S$ for all $R \in K$ and

$$\begin{aligned} S \text{ nullspace } & \left[\sum_R \chi^*(R) \Gamma(R) \right] \\ & = \text{nullspace } \left[\sum_R \chi^*(R) \Gamma'(R) \right]. \end{aligned} \quad (3.12)$$

For a given arithmetic point group $\Gamma(R)$ with given $D_I(K)$ one can determine all space groups. Two space groups from this set are equivalent if there is an element of the normalizer which satisfies (3.12) for $\Gamma'(K) = \Gamma(K)$ and which maps the translation parts of G to the corresponding ones of G' , modulo lattice translations and origin shifts.

In particular, when D_E and D_I are irreducible and non-equivalent, the situation simplifies. An element S of the centralizer is equivalent to the direct sum of multiples of the identity in both V_E and V_I . Therefore, both spaces are left invariant by S and (3.12) is satisfied. An element S of the normalizer gives an automorphism Φ of the group K . If $D_E[\Phi(K)]$ is equivalent to $D_E(K)$, (3.12) is satisfied. Otherwise V_E and V_I are interchanged and (3.12) is violated.

The third case is that of a mixed point group. In that case the distinct space V_E is not left invariant by the point group. Since no such systems are known at present, we shall skip their discussion.

4. Self-similarity

4.1. Self-similarity in one-dimensional systems

Tilings and quasicrystals may have an additional symmetry property that is not present (or only trivially) in periodic crystals: scale invariance. Consider the diffraction pattern of a quasiperiodic system. If there is a number λ such that for every vector of the Fourier module its λ multiple belongs also to the module, it means that M^* has scale invariance. One can associate an integer matrix $\Gamma(S)$ to this transformation:

$$\lambda \mathbf{a}_i^* = \sum_{j=1}^n \Gamma^*(S)_{ji} \mathbf{a}_j. \quad (4.1)$$

The dual mapping $\Gamma(S)$ maps Σ to itself. When is such a scale invariance present? Consider first a one-dimensional tiling of rank 2 and a basis transformation P of the lattice Σ . P has determinant $D = \pm 1$ and integer trace n . Then its eigenvalues are

$$\lambda_{1,2} = (n/2) \pm \frac{1}{2}(n^2 - 4D)^{1/2}. \quad (4.2)$$

The eigenspace corresponding to λ_j is V_j . Then $V_s =$

$V_1 \oplus V_2$. With this decomposition two vectors (a, b) and $(\lambda_1 a, \lambda_2 b)$ span a lattice. This lattice can be chosen to be orthogonal or isometric. If $D = -1$, one has $\lambda_2 = -\lambda_1^{-1} \equiv -\lambda^{-1}$. Then $\{(a, \lambda a), (\lambda a - a)\}$ spans a square lattice. If $D = +1$, one has $\lambda_2 = \lambda_1^{-1} = \lambda$. Then $\{(a, \lambda a), (\lambda a, a)\}$ spans a lattice with basis vectors of equal length. With the choice $b = a\lambda^{1/2}$, the basis $(a, a\lambda^{1/2}), (\lambda a - a, a/\lambda^{1/2} - a\lambda^{1/2})$ is orthogonal. A tiling obtained from this lattice by attaching line elements perpendicular to V_1 is, by construction, invariant under a scaling transformation with factor λ (4.2). For $D = -1$, the incommensurability of the Fourier module (the ratio of two basis vectors modulo 1) is λ . This is also the case for the isometric lattice for $D = \pm 1$.

V_E is the eigenspace for λ and V_I that for D/λ . If λ is the eigenvalue (4.2) with the largest absolute value, P dilates V_s along V_E and contracts it along V_I . A vertex of Σ for which the atomic surface intersects V_E will be mapped to a vertex with a smaller distance to V_E , which will, therefore, also give a vertex of the tiling. So each of the tiling vertices is mapped to another one, which means self-similarity. It is not even necessary that P be a basis transformation. Any integral matrix with $|\lambda_1| > 1$ and $|\lambda_2| < 1$ gives a self-similar tiling. If the trace and determinant of P are denoted by n and D , respectively, this is the case for $|n| > |D+1|$. So there is a dense set of 1D rank two tilings with self-similarity.

The orbits of the vertices of Σ under a self-similarity transformation lie on hyperbolae. Sometimes, there is a metrical tensor that is left invariant. On the basis of $V_E \oplus V_I$, the condition for this is

$$\begin{pmatrix} \lambda & 0 \\ 0 & D/\lambda \end{pmatrix} \begin{pmatrix} a & b \\ b & c \end{pmatrix} \begin{pmatrix} \lambda & 0 \\ 0 & D/\lambda \end{pmatrix} = \begin{pmatrix} a & b \\ b & c \end{pmatrix}. \quad (4.3)$$

This happens only if $D = \pm 1$ and $a = c = 0$. In that case the self-similarity transformations of the tiling correspond to a Minkowski transformation in V_s which leaves an indefinite metrical tensor invariant (Janner, 1988).

4.2. Self-similarity for systems with dimensions 2 and 3

The self-similarity of quasiperiodic tilings in a space of dimension larger than one is related to the point-group symmetry, because the origin of the isotropy of the scaling transformation is this symmetry. For simplicity we assume here that the n -dimensional point group $\Gamma(K)$ has two physically non-equivalent irreducible components of the same dimension. Then consider an element S from the centralizer of $\Gamma(K)$, i.e. a non-singular integer matrix such that $S\Gamma(R) = \Gamma(R)S$ for every $R \in K$. Because of Schur's lemma S is the direct sum of multiples of the identity in both subspaces. Because it is nonsingular S is equivalent to $\lambda 1_E \oplus (\pm \lambda^{-1} 1_I)$. For a tiling with point group $\Gamma(K)$, which can be obtained by the intersection with

V_E of atomic surfaces parallel to V_I , this means self-similarity with a factor λ .

This is the situation for the standard pentagonal, octagonal, decagonal, dodecagonal and icosahedral tilings. As an example, consider the point group of the standard octagonal tiling. It is generated by R_1 and R_2 and has an element $\Gamma(S)$ of the centralizer:

$$\begin{aligned} \Gamma(R_1) &= \begin{pmatrix} 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \\ \Gamma(R_2) &= \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \\ \Gamma(S) &= \begin{pmatrix} 1 & 1 & 0 & -1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ -1 & 0 & 1 & 1 \end{pmatrix}. \end{aligned} \tag{4.4}$$

The matrix $\Gamma(S)$ has two eigenvalues $1 + 2^{1/2}$ and two eigenvalues $1 - 2^{1/2}$. Their eigenspaces are V_E and V_I , respectively. This implies that the tiling is invariant under S , which is a scale transformation with factor $1 + 2^{1/2}$ (Fig. 6).

If $\Gamma(S)$ is an element of the normalizer, it induces an automorphism π . Similarly to what has been said in §3, D_E may or may not be equivalent to $D_E\pi$. In

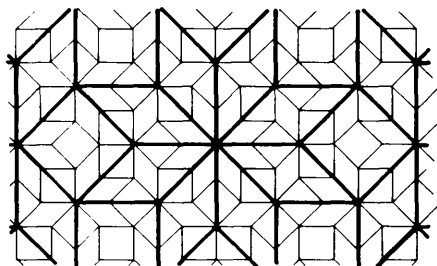


Fig. 6. Standard octagonal tiling with self-similarity factor $1 + 2^{1/2}$.

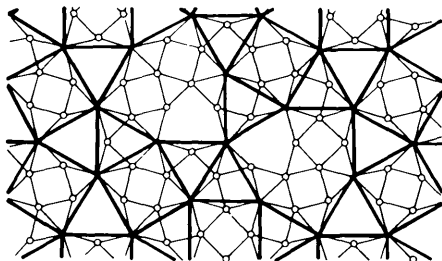


Fig. 7. A dodecagonal tiling with self-similarity transformation consisting of a dilation $(2 + 3^{1/2})^{1/2}$ and a rotation over $\pi/12$.

the former case it follows from Schur's lemma that S leaves both V_E and V_I invariant; and there is again an associated self-similarity transformation. If D_E is not equivalent with $D_E\pi$ there is no such transformation, because then S interchanges V_E and V_I .

In the former case S leaves V_E invariant, but it is, generally, not a multiple of the identity. Consider as an example a dodecagonal point group. Its generators $\Gamma(R_1)$ and $\Gamma(R_2)$ and an element of the normalizer are

$$\begin{aligned} \Gamma(R_1) &= \begin{pmatrix} 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \\ \Gamma(R_2) &= \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \\ \Gamma(S) &= \begin{pmatrix} 1 & 0 & 0 & -1 \\ 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}. \end{aligned} \tag{4.5}$$

$\Gamma(S)$ induces an automorphism π that sends R_1 to R_1 and R_2 to $R_1^{-1}R_2$. It has four complex eigenvalues $\lambda, \lambda^*, \lambda^{-1}, \lambda^{*-1}$ with $\lambda = 2 + 3^{1/2} \exp(\pi/12)$ and V_E belongs to the eigenvalues λ and λ^* . Therefore, the action of S on the 2D dodecagonal tiling is a scale transformation with factor $(2 + 3^{1/2})^{1/2}$ followed by a rotation over 15° (Fig. 7). This is in fact the symmetry of a spiral.

As in the one-dimensional case it is not necessary that S has determinant equal to ± 1 . If $\Gamma(S)$ is an integer matrix such that it commutes with every $\Gamma(R)$ in $\Gamma(K)$ it also gives rise to a scale transformation (Janssen, 1990). A matrix $\Gamma(S)$ with determinant different from one in absolute value corresponds to a centring of the lattice.

These scale transformations do not leave the physical laws invariant. Nevertheless they play a role in the structure. They are directly related to the inflation and deflation rules used to construct tilings. Furthermore, scale invariance has been shown to be of importance when studying electrons in a quasiperiodic chain. Finally, they are the same symmetry transformations that play a role in regular fractals.

5. Scale-space groups

In the preceding sections we have studied the crystallographic distance-preserving symmetries of quasiperiodic structures and their scaling properties. Both types of symmetry transformations can also be combined, just as one can combine rotations and

translations to Euclidean transformations. In this way one sometimes gets non-trivial results, comparable to the non-trivial combination of lattice translations and rotations in a non-symmorphic space group.

The procedure is the same. Suppose $\Gamma(K)$ is generated by $\{\Gamma(R_i)\}$, and the group of scale transformations by $\{\Gamma(S_j)\}$. They satisfy relations $\Phi_\mu(R_1, \dots, S_1, \dots) = E$. One chooses the affine transformations $\{R|\mathbf{t}_R\}$ in such a way that as many as possible components of \mathbf{t}_R are zero, using a shift of origin. Then the relations $\Phi_\mu(\{R_1|\mathbf{t}_{R_1}\}, \dots, \{S_1|\mathbf{t}_S\}, \dots) = \{1|0\}$ give the sufficient and necessary conditions for the non-primitive translations $\mathbf{t}_{R,S}$.

Consider as an example the infinite group generated by

$$\Gamma(R) = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \Gamma(S) = \begin{pmatrix} 3 & 2 \\ 2 & 1 \end{pmatrix}. \quad (5.1)$$

The second matrix gives a self-similarity transformation with factor $3+2\tau$, where $\tau = (5^{1/2} - 1)/2$. The group generated by $\Gamma(R)$ only has trivial extensions because, since $\det[E - \Gamma(R)] \neq 0$, there is an origin such that $\mathbf{t}_R = 0$. The same holds for the group generated by $\Gamma(S)$. For the group generated by (5.1), one may again choose $\mathbf{t}_R = 0$, but then no freedom is left for changing \mathbf{t}_S . In fact, we have chosen the origin in a centre of inversion. If $\mathbf{t}_S = (a, b)$ it follows from the relations $R^2 = E$, $SR = RS$ that $(a, b) - (a, b) \equiv 0 \pmod{1}$ and that $(-a, b) \equiv (a, b)$. Therefore, there are four non-equivalent extensions, corresponding to $(a, b) = (0, 0)$, $(\frac{1}{2}, 0)$, $(0, \frac{1}{2})$ and $(\frac{1}{2}, \frac{1}{2})$, respectively. By a proper choice of basis the last three can be identified. So there exist non-trivial scale-space groups. They may lead to scale-invariant decorations (Janner & Janssen, 1990), but it is not clear whether they have relevance for physical properties.

6. Concluding remarks

To describe the symmetry of quasiperiodic structures, one has to revise the crystallographic notions. Because quasiperiodic structures are restrictions of periodic structures to physical space, one may consider the higher-dimensional space group of that periodic structure as the symmetry of the quasiperiodic structure. As a matter of fact, relations between spot intensities and systematic extinctions which are pres-

ent in the higher-dimensional structure as a consequence of the space group are also present for the quasiperiodic structure, because the Fourier module is the projection of the reciprocal lattice Σ^* .

An n -dimensional space-group element acts on the physical structure as a distance-preserving transformation plus a compensating transformation in internal space. For a modulated structure a translation in internal space is just a symmetry-restoring phase shift of the modulation. In general, the internal transformation is analogous to a gauge transformation. This has been discussed by Janner & Janssen (1977).

For a quasiperiodic structure with rank exceeding the dimension, the intersection points of planes parallel to V_E , going through the lattice points of Σ , form a dense set. For any two points from this set, there is a translation for which the internal part connects them. In physical space the system is just shifted over the external part of the translation. Such a shift keeps the physics the same. The same is true for an n -dimensional reducible space-group element. Generally, it is not true for other groups, like scale-space groups or groups with a mixing point group. Such transformations may nevertheless have observable consequences.

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