$$f(x_1, \ldots, x_n) = \sum_{m_1} \ldots \sum_{m_n} A_{m_1,\ldots,m_n} \exp[2\pi i(m_1 x_1 + \ldots + m_n x_n)] \tag{1.10.1.15}$$

and consequently

$$g(x) = \sum_{m_1 \ldots m_n} A_{m_1,\ldots,m_n} \exp\left[2\pi i\left(\sum_{i=1}^{n} m_i \alpha_i\right)x\right], \tag{1.10.1.16}$$

which proves that the function is quasiperiodic of rank $n$ with $n$ reciprocal-basis vectors $2\pi\alpha_i$ in one dimension.

The quasiperiodic function $g(x)$ is therefore the restriction to the line $(\alpha_1 x, \ldots, \alpha_n x)$ in $n$-dimensional space. This is a general situation. Each quasiperiodic function can be obtained as the restriction of a periodic function in $n$ dimensions to a subspace that can be identified with the physical space. We denote the $n$-dimensional space in which one finds the lattice periodic structure (the *superspace*) by $V_s$, the *physical space* by $V_E$ and the additional space, called *internal space*, by $V_I$, such that $V_s$ is the direct sum of $V_E$ and $V_I$. In the field of quasicrystals, one often uses the name *parallel space* for $V_E$ and *perpendicular space* for $V_I$.

On the other hand, one can embed the quasiperiodic function in superspace, which means that one constructs a lattice periodic function in $n$ dimensions such that its restriction to physical space is the quasiperiodic function. Take as an example the displacively modulated structure of equation (1.10.1.2). Compare this three-dimensional structure with the array of lines

$$\big(\mathbf{n} + \mathbf{r}_j + \mathbf{f}_j(\mathbf{Q}\cdot\mathbf{n} + t), t\big) \quad (\text{real } t) \tag{1.10.1.17}$$

in four-dimensional space. The restriction to the three-dimensional hyperplane $t = 0$ gives exactly the structure (1.10.1.2). Moreover, the four-dimensional array of lines is lattice periodic. Because $\mathbf{f}_j$ is periodic, the array is left invariant if one replaces $t$ by $t + 1$, and for every lattice vector $\mathbf{m}$ of the basic structure the array is left invariant if one replaces simultaneously $t$ by $t - \mathbf{Q}\cdot\mathbf{m}$. This means that the array is left invariant by all four-dimensional lattice vectors of the lattice $\Sigma$ with basis

$$\mathbf{a}_{si} = (\mathbf{a}_i, -\mathbf{Q}\cdot\mathbf{a}_i) \quad (i = 1, 2, 3), \quad \mathbf{a}_4 = (0, 1). \tag{1.10.1.18}$$

Indeed the quasiperiodic IC phase is the restriction to $V_E$ $(t = 0)$ of the lattice periodic function in four dimensions.

The reciprocal basis for (1.10.1.18) consists of the basis vectors

$$\mathbf{a}^*_{si} = (\mathbf{a}^*_i, 0) \quad (i = 1, 2, 3), \quad \mathbf{a}^*_4 = (\mathbf{Q}, 1). \tag{1.10.1.19}$$

These span the reciprocal lattice $\Sigma^*$. The projection of this basis on $V_E$ consists of the four vectors $\mathbf{a}^*_i$ $(i = 1, 2, 3)$ and $\mathbf{Q}$, and these form the basis for the Fourier module of the quasiperiodic structure.

This is a well known situation. From the theory of Fourier transformation one knows that the projection of the Fourier transform of a function in $n$ dimensions on a $d$-dimensional subspace is the Fourier transform of the restriction of that $n$-dimensional function to the same $d$-dimensional subspace. This gives a way to embed the quasiperiodic structure in a space with as many dimensions as the rank of the Fourier module. One considers the basis of the Fourier module as the projection of $n$ linearly independent vectors in $n$-dimensional space. This means that for every vector of the Fourier module one has exactly one reciprocal-lattice vector in $V_s$. Suppose the quasiperiodic structure is given by some function, for example the density $\rho(\mathbf{r})$. Then

$$\rho(\mathbf{r}) = \sum_{\mathbf{H}\in M^*} \hat{\rho}(\mathbf{H}) \exp(i\mathbf{H}\cdot\mathbf{r}). \tag{1.10.1.20}$$

One may define a function in $n$-dimensional space by

$$\rho_s(\mathbf{r}_s) = \sum_{\mathbf{H}_s\in\Sigma^*} \hat{\rho}(\mathbf{H}) \exp(i\mathbf{H}_s\cdot\mathbf{r}_s), \tag{1.10.1.21}$$

where $\mathbf{H}_s$ is the unique reciprocal-lattice vector that is projected on the Fourier module vector $\mathbf{H}$. It is immediately clear that the restriction of $\rho_s$ to physical space is exactly $\rho$. Moreover, the function $\rho_s$ is lattice periodic with lattice $\Sigma$, for which $\Sigma^*$ is the reciprocal lattice.

This construction can be performed in the following equivalent way. Consider a point $\mathbf{r}$ in physical space, where one has the quasiperiodic function $\rho(\mathbf{r})$. The Fourier module of this function is the projection on physical space of the $n$-dimensional reciprocal lattice $\Sigma^*$ with basis vectors $\mathbf{a}^*_{si}$ $(i = 1, 2, \ldots, n)$. The reciprocal lattice $\Sigma^*$ corresponds to the direct lattice $\Sigma$. A point $\mathbf{r}$ in $V_E$ can also be considered as an element $(\mathbf{r}, 0)$ in $n$-dimensional space. By the translations of $\Sigma$, this point is equivalent with a point $\mathbf{r}_s$ with lattice coordinates

$$\xi_i = \text{Frac}(\mathbf{a}^*_{si}.(\mathbf{r}, 0)) = \text{Frac}(\mathbf{a}^*_i\cdot\mathbf{r}) \tag{1.10.1.22}$$

in the unit cell of $\Sigma$, where $\text{Frac}(x)$ is $x$ minus the largest integer smaller than $x$. If one puts $\rho_s(\mathbf{r}_s) = \rho(\mathbf{r})$, the function $\rho$ determines the function $\rho_s$ in the unit cell, and consequently in the whole $n$-dimensional space $V_s$. This means that all the information about the structure in $V_E$ is mapped onto the information inside the $n$-dimensional unit cell. *The information in three dimensions is exactly the same as that in superspace*. Only the presentation is different.

In the case in which the crystal consists of point atoms, the corresponding points in $d$-dimensional physical space $V_E$ are the intersection of $(n - d)$-dimensional hypersurfaces with $V_E$. For displacively modulated IC phases in three dimensions with one modulation wavevector, one has $n = 4$, $d = 3$ and the hypersurfaces are just lines in superspace, as we have seen. For more independent modulation vectors the dimension of the hypersurfaces is larger than one. In this case, as often in the case of composite structures, the $(n - d)$-dimensional surfaces do not have borders. This in contrast to quasicrystals, where they are bounded. All these hypersurfaces for which the intersection with physical space gives the atomic positions are called *atomic surfaces*.

Physical properties of aperiodic but quasi-periodic structures are partly determined by their symmetry, which can be formulated using the superspace approach. Here we deal mainly with such symmetry-related properties. A more extensive view is given in Janssen *et al.* (2007).

## 1.10.2. Symmetry

### 1.10.2.1. *Symmetry transformations*

Because the embedded periodic structure in $n$ dimensions has lattice periodicity, it has $n$-dimensional space-group symmetry as well. It is not *a priori* clear that such a symmetry group in the unphysical $n$-dimensional space is relevant for the physical structure, but we shall show here that the superspace description is indeed useful for the description of quasiperiodic systems. First we shall discuss some of the structures of these higher-dimensional space transformations.

Suppose the diffraction pattern has rotational symmetry. Consider for example an orthogonal transformation $R$ that leaves the diffraction pattern invariant. In particular, any basis vector of the module is transformed into an element of the module, *i.e.* an integral linear combination of the basis vectors.

$$R\mathbf{a}^*_i = \sum_{j=1}^{n} M_{ji}\mathbf{a}^*_j, \quad i = 1, 2, \ldots, n. \tag{1.10.2.1}$$

Because the matrix $M$ depends on $R$ and acts in reciprocal space, we denote it by $\Gamma^*(R) = M$. The matrix $\Gamma^*(R)$ has integer entries. Because the intensity of the diffraction pattern is not constant on circles around the origin (that would imply that one can not distinguish separate peaks), the orthogonal transformation $R$ is of

finite order. Then a theorem from group theory states that $\Gamma^*(R)$ is similar to an $n$-dimensional orthogonal transformation $R_s$. The latter certainly has an invariant subspace: the physical space. Therefore, one can find a basis transformation $S$ such that the matrix $\Gamma^*(R)$ is conjugated to the direct sum of an orthogonal transformation $R$ in $V_E$ and an additional orthogonal transformation in $V_I$:

$$S\Gamma^*(R)S^{-1} = \begin{pmatrix} R & 0 \\ 0 & R_I \end{pmatrix}, \quad R \in O(d), \quad R_I \in O(n-d). \tag{1.10.2.2}$$

We denote this orthogonal transformation in $V_s$ as $R_s$ or as a couple $(R, R_I)$. Clearly, the transformation $R_s$ leaves the embedded reciprocal lattice $\Sigma^*$ invariant. Moreover, this transformation leaves the direct lattice $\Sigma$ invariant as well. As always, the action of $R_s$ on the basis of $\Sigma$ for which $\mathbf{a}^*_{si}$ form the reciprocal basis is then given by

$$R_s\mathbf{a}_{si} = \sum_{j=1}^{n} \Gamma(R)_{ji}\mathbf{a}_{sj} \;\text{ with }\; \Gamma(R)_{ij} = \Gamma^*(R^{-1})_{ji}. \tag{1.10.2.3}$$

This is the usual relation between the action on a basis and the action on the reciprocal basis.

By construction, the orthogonal transformation $R_s = (R, R_I)$ leaves the lattice $\Sigma$ invariant, and can therefore belong to the point group of a periodic structure with this lattice. In general, such a point-group element does not leave the periodic structure itself invariant, just as a point group in three dimensions does not leave a crystal with a nonsymmorphic space group invariant. One then has to combine the orthogonal transformation with a translation that in general does not belong to the lattice. Here a translation has components in physical as well as in internal space. A translation can be denoted by $(\mathbf{a}_E, \mathbf{a}_I)$. Then a general solid motion can be written as

$$g = \big\{(R, R_I)|(\mathbf{a}_E, \mathbf{a}_I)\big\}. \tag{1.10.2.4}$$

The action of such a transformation on a point $r_s$ in superspace is given by

$$gr_s = g(\mathbf{r}_E, \mathbf{r}_I) = (R\mathbf{r}_E + \mathbf{a}_E, R_I\mathbf{r}_I + \mathbf{a}_I). \tag{1.10.2.5}$$

If such a transformation leaves the periodic array of atomic surfaces in superspace invariant, it is a symmetry transformation. In particular, the elements $(\mathbf{a}_E, \mathbf{a}_I)$ of the translation group $\Sigma$ are such symmetry transformations.

### 1.10.2.2. *Point groups*

The orthogonal transformations that leave the diffraction pattern invariant form a point group $K$, a finite subgroup of $O(d)$, where $d$ is the dimension of the physical space. All elements act on the basis of the Fourier module as in (1.10.2.1) and the matrices $\Gamma^*(K)$ form a representation of the group $K$, an integral representation because the matrices have all integer entries, and reducible because the physical space is an invariant subspace for $\Gamma^*(K)$. Because $K$ is finite, this representation is equivalent with a representation in terms of orthogonal matrices. Moreover, by construction $\Gamma^*(K)$ leaves the $n$-dimensional reciprocal lattice $\Sigma^*$ invariant. It is an $n$-dimensional crystallographic point group. The components $R$ of $R_s$ form a $d$-dimensional point group $K_E$, which is not necessarily crystallographic, and the components $R_I$ form an $(n-d)$-dimensional point group $K_I$.

Consider as an example an IC phase with orthorhombic basic structure and one independent modulation wavevector $\gamma\mathbf{c}^*$ along the $c$ axis. Suppose that the Fourier module, which is of rank four, is invariant under the point group $mmm$. Then one has for the three generators

$$\begin{array}{llll} m_x\mathbf{a}^*_1 = -\mathbf{a}^*_1, & m_x\mathbf{a}^*_2 = \mathbf{a}^*_2, & m_x\mathbf{a}^*_3 = \mathbf{a}^*_3, & m_x\mathbf{a}^*_4 = \mathbf{a}^*_4 \\ m_y\mathbf{a}^*_1 = \mathbf{a}^*_1, & m_y\mathbf{a}^*_2 = -\mathbf{a}^*_2, & m_y\mathbf{a}^*_3 = \mathbf{a}^*_3, & m_y\mathbf{a}^*_4 = \mathbf{a}^*_4 \\ m_z\mathbf{a}^*_1 = \mathbf{a}^*_1, & m_z\mathbf{a}^*_2 = \mathbf{a}^*_2, & m_z\mathbf{a}^*_3 = -\mathbf{a}^*_3, & m_z\mathbf{a}^*_4 = -\mathbf{a}^*_4. \end{array}$$

Therefore, the corresponding matrices $\Gamma^*(R)$ are

$$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \tag{1.10.2.6}$$

which implies that the three generators of the four-dimensional point group are $(m_x, 1)$, $(m_y, 1)$ and $(m_z, \bar{1})$.

The diffraction pattern of the standard octagonal tiling has rank four, basis vectors of the Fourier module are

$$(1, 0), \quad (\sqrt{1/2}, \sqrt{1/2}), \quad (0, 1), \quad (-\sqrt{1/2}, \sqrt{1/2})$$

and the pattern is invariant under a rotation of $\pi/4$ and a mirror symmetry. The action of these elements on the given basis of the Fourier module is

$$\Gamma^*(R_1) = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad \Gamma^*(R_2) = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

By a basis transformation, one may bring these transformations into the form

$$\begin{pmatrix} \cos(\pi/4) & -\sin(\pi/4) & 0 & 0 \\ \sin(\pi/4) & \cos(\pi/4) & 0 & 0 \\ 0 & 0 & \cos(3\pi/4) & -\sin(3\pi/4) \\ 0 & 0 & \sin(3\pi/4) & \cos(3\pi/4) \end{pmatrix}, \quad \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Therefore, the $\pi/4$ rotation in physical space is combined with a $3\pi/4$ rotation in internal space in order to get a transformation that leaves a lattice invariant.

A three-dimensional example is the case of a quasicrystal with icosahedral symmetry. For the diffraction pattern all spots may be labelled with six indices with respect to a basis with basis vectors

$$\begin{aligned} \mathbf{a}^*_1 &= (0, 0, 1) \\ \mathbf{a}^*_2 &= (a, 0, b) \\ \mathbf{a}^*_3 &= (a\cos(2\pi/5), a\sin(2\pi/5), b) \\ \mathbf{a}^*_4 &= (a\cos(4\pi/5), a\sin(4\pi/5), b) \\ \mathbf{a}^*_5 &= (a\cos(4\pi/5), -a\sin(4\pi/5), b) \\ \mathbf{a}^*_6 &= (a\cos(2\pi/5), -a\sin(2\pi/5), b), \end{aligned}$$

with $a = 2/\sqrt{5}$ and $b = 1/\sqrt{5}$. The rotation subgroup that leaves the Fourier module invariant is generated by

$$\Gamma^*(A) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\Gamma^*(B) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}. \quad (1.10.2.7)$$

Moreover, there is the central inversion $-E$. The six-dimensional representation of the symmetry group, which is the icosahedral group $\bar{5}\bar{3}m$, is reducible into the sum of two nonequivalent three-dimensional irreducible representations. A basis for this representation in the six-dimensional space is then given by

$$\begin{matrix} (\mathbf{a}_1^*, c\mathbf{a}_1^*) & (\mathbf{a}_2^*, -c\mathbf{a}_2^*) & (\mathbf{a}_3^*, -c\mathbf{a}_4^*) \\ (\mathbf{a}_4^*, -c\mathbf{a}_6^*) & (\mathbf{a}_5^*, -c\mathbf{a}_3^*) & (\mathbf{a}_6^*, -c\mathbf{a}_5^*), \end{matrix} \quad (1.10.2.8)$$

which projects on the given basis in $V_E$.

The point-group elements considered here are pairs of orthogonal transformations in physical and internal space. Orthogonal transformations that do not leave these two spaces invariant have not been considered. The reason for this is that the information about the reciprocal lattice comes from its projection on the Fourier module in physical space. By changing the length scale in internal space one does not change the projection but one would break a symmetry that mixes the two spaces. Nevertheless, quasicrystals are often described starting from an $n$-dimensional periodic structure with a lattice of higher symmetry. For example, the icosahedral 3D Penrose tiling can be obtained from a structure with a hypercubic six-dimensional lattice. Its reciprocal lattice is that spanned by the vectors (1.10.2.8) where one puts $c = 1$. The symmetry of the periodic structure, however, is lower than that of the lattice and has a point group in reducible form. Therefore, we shall consider here only reducible point groups, subgroups of the orthogonal group $O(n)$ which have a $d$-dimensional invariant subspace, identified with the physical space.

The fact that the spaces $V_E$ and $V_I$ are usually taken as mutually perpendicular does not have any physical relevance. One could as well consider oblique projections of a reciprocal lattice $\Sigma^*$ on $V_E$. What is important is that the intersection of the periodic structure with the physical space should be the same in all descriptions. The metric in internal space $V_I$ follows naturally from the fact that there is a finite group $K_I$.

### 1.10.2.3. *Superspace groups*

The quasiperiodic function $\rho(\mathbf{r})$ in $d$ dimensions can be embedded as lattice periodic function $\rho_s(\mathbf{r}_s)$ in $n$ dimensions. The symmetry group of the latter is the group of all elements $g$ (1.10.2.4) for which

$$\rho_s(\mathbf{r}_s) = \rho_s(g\mathbf{r}_s) = \rho_s(R_E\mathbf{r} + \mathbf{a}_E, R_I\mathbf{r}_I + \mathbf{a}_I). \quad (1.10.2.9)$$

This group is an $n$-dimensional space group $G$. It has an invariant subgroup of translations, which is formed by the lattice translations $\Sigma$, and the quotient $G/\Sigma$ is isomorphic to the $n$-dimensional point group $K$. However, not every $n$-dimensional space group can occur here because we made the restriction to reducible point groups. For example, the $n$-dimensional hypercubic groups do not occur in this way as symmetry groups of quasiperiodic systems.

The product of two superspace group elements is

$$\{R_{s1}|\mathbf{a}_{s1}\}\{R_{s2}|\mathbf{a}_{s2}\} = \{R_{s1}R_{s2}|\mathbf{a}_{s1} + R_{s1}\mathbf{a}_{s2}\}. \quad (1.10.2.10)$$

On a lattice basis for $\Sigma$, the orthogonal transformations $R_{s1}$ and $R_{s2}$ are integer $n \times n$ matrices and the translations $\mathbf{a}_{s1}$ and $\mathbf{a}_{s2}$ are column vectors. The orthogonal transformations $R_s$ leave the origin invariant. The translations depend on the choice of this origin. For a symmorphic space group there is a choice of origin such that the translations $a$ are lattice translations.

The point-group elements are reducible, which means that in the physical space one has the usual situation. If $d = 3$ then the only intrinsic nonprimitive translations are those in screw axes or glide planes. An $n$-dimensional orthogonal transformation can always be written as the sum of a number $r$ of two-dimensional rotations with rotation angle different from $\pi$, a $p$-dimensional total inversion and a $q$-dimensional identity transformation. The integers $r$, $p$, $q$ may be zero and $2r + p + q = n$. The possible intrinsic nonprimitive translations belong to the $q$-dimensional space in which the identity acts. For the three examples in the previous section, the internal component of the nonprimitive translation for $m_x$ and $m_y$ in the first example can be different from zero, but that for $m_z$ in the same example is zero. For the octagonal case, only the second generator can have an intrinsic nonprimitive translation in the fourth direction, and for the icosahedral case the two generators have one two-dimensional invariant plane and one pointwise invariant line in $V_I$.

In the diffraction pattern of an IC phase one can distinguish between main reflections and satellites. A symmetry operation cannot transform a main reflection into a satellite. This implies that for these structures the reciprocal lattice of the basic structure is left invariant by the point group, and consequently the latter must be a three-dimensional crystallographic point group. Therefore, the point groups for IC phases are the same as those for lattice periodic systems. They act in superspace as a representation of a three-dimensional crystallographic point group. This is not true for an arbitrary quasiperiodic structure. The restriction in the general case comes from the requirement that the three-dimensional point group must have a faithful integer matrix representation in superspace. There is a mathematical statement to the effect that the lowest dimension in which a $p$-fold rotation can be represented as an integer matrix is given by the Euler function, the number of integers smaller than $p$ that do not divide $p$. For example, for a prime number $p$ this number is $p - 1$. This implies that if one restricts the rank of the Fourier module (*i.e.* the dimension of the superspace) to six, only values 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 12, 14 and 18 are possible for $p$. The values 7, 9, 14 and 18 only occur for two-dimensional quasiperiodic structures of rank six. Therefore, the allowable three-dimensional point groups for systems up to rank six are limited to the groups given in Table 1.10.2.1. The possible superspace groups for IC modulated phases of rank four are given in Chapter 9.8 of Volume C of *International Tables* (2004). Superspace groups for quasicrystals of rank $n \leq 6$ are given in Janssen (1988).

The notation of higher-dimensional symmetry groups is discussed in two IUCr reports (Janssen *et al.*, 1999, 2002).

### 1.10.2.4. *Magnetic superspace groups*

Just as for point groups and space groups for lattice periodic systems, one may generalize the symmetry groups to magnetic groups for general quasi-periodic structures (*c.f.* Section 1.2.5). Time reversal comes in for magnetic superspace groups. Just as three-dimensional space groups give rise to magnetic space groups (see Section 1.2.5), superspace groups give rise to magnetic superspace groups (Janner & Janssen, 1980). Consider a basic structure with space group *Pmmm*. Suppose that there

Table 1.10.2.1. *Allowable three-dimensional point groups for systems up to rank six*

| Isomorphism class | Order | Three-dimensional point groups |
|---|---|---|
| $C_1$ | 1 | 1 |
| $C_2$ | 2 | 2, $\bar{1}$, $m$ |
| $C_3$ | 3 | 3 |
| $C_4$ | 4 | 4, $\bar{4}$ |
| $C_5$ | 5 | 5 |
| $C_6$ | 6 | 6, $\bar{6}$, $\bar{3}$ |
| $C_8$ | 8 | 8, $\bar{8}$ |
| $C_{10}$ | 10 | 10, $\bar{10}$, $\bar{5}$ |
| $C_{12}$ | 12 | 12, $\bar{12}$ |
| $D_2$ | 4 | 222, $2/m$, $2mm$ |
| $D_3$ | 6 | 32, $3m$ |
| $D_4$ | 8 | 422, $4mm$, $\bar{4}2m$ |
| $D_5$ | 10 | 52, $5m$ |
| $D_6$ | 12 | 622, $\bar{3}m$, $6mm$, $\bar{6}2m$ |
| $D_8$ | 16 | 822, $8mm$, $\bar{8}2m$ |
| $D_{10}$ | 20 | 10 22, 10 $mm$, $\bar{10}$ $2m$, $\bar{5}m$ |
| $D_{12}$ | 24 | 12 22, 12 $mm$, $\bar{12}$ $2m$ |
| $C_4 \times C_2$ | 8 | $4/m$ |
| $C_6 \times C_2$ | 12 | $6/m$ |
| $C_8 \times C_2$ | 16 | $8/m$ |
| $C_{10} \times C_2$ | 20 | $10/m$ |
| $C_{12} \times C_2$ | 24 | $12/m$ |
| $D_2 \times C_2$ | 8 | $mmm$ |
| $D_4 \times C_2$ | 16 | $4/mmm$ |
| $D_6 \times C_2$ | 24 | $6/mmm$ |
| $D_8 \times C_2$ | 32 | $8/mmm$ |
| $D_{10} \times C_2$ | 40 | $10/mmm$ |
| $D_{12} \times C_2$ | 48 | $12/mmm$ |
| $T$ | 12 | 23 |
| $O$ | 24 | 432, $\bar{4}3m$ |
| $I$ | 60 | 532 |
| $T \times C_2$ | 24 | $m\bar{3}$ |
| $O \times C_2$ | 48 | $m\bar{3}m$ |
| $I \times C_2$ | 120 | $\bar{5}\bar{3}m$ |

exists a spin wave with wave vector $\gamma\mathbf{c}^*$ and with spins pointing in the $a$ direction.

$$\mathbf{S}(\mathbf{n}, j) = \mathbf{S}_j \cos(\gamma\mathbf{c}^* \cdot \mathbf{n}), \tag{1.10.2.11}$$

with $\mathbf{S}_j$ parallel to $\mathbf{a}$ for $j = 1$. The superspace group is $Pmmm(00\gamma)$. Element $m_x$ leaves the spin wave invariant, $m_y$ and $m_z$ invert the spin. Introducing the time reversal $\theta$, the spin wave is left invariant by $m_x$, $m_y\theta$ and $m_z\theta$. The spin wave in superspace is given by

$$\mathbf{S}(\mathbf{n}, j, t) = \mathbf{S}_j \cos(\gamma\mathbf{c}^* \cdot \mathbf{n} + 2\pi t). \tag{1.10.2.12}$$

An obvious additional symmetry element then is the shift in internal space ($t \rightarrow t + 1/2$) combined with $\theta$. However, the situation is different when one also considers the modulation of the nuclear structure. If, for example by spin-lattice coupling, the latter has a modulation function $\mathbf{u}(\mathbf{n}, j, t) = \mathbf{u}_j \cos(\gamma\mathbf{c}^* \cdot \mathbf{n} + 2\pi t)$ in superspace, this function changes sign under $t \rightarrow t + 1/2$, and is invariant under $\theta$. Then $(\theta|0001/2)$ is not a symmetry element.

As for two- and three-dimensional magnetic space groups, there are four types of groups associated with a given superspace group. If no element appears containing time reversal, one has a non-magnetic superspace group. If pure time reversal is an element, the group is a grey group and is the direct product of a non-magnetic superspace group with the group of two elements consisting of $\theta$ and the identity. The others are black-and-white groups. The subgroup of primed and unprimed elements (pure translations or products of a translation and time reversal) may have only unprimed elements (type 3) or have also primed elements (type 4). In the latter case the unprimed elements form a subgroup of index 2. The symbol for the magnetic superspace group is the symbol for the superspace group of unprimed elements, with an additional $1'$ after the symbol (for type 2), primes on all point-group elements associated with time reversal (type 3), or an additional subindex indicating a primed translation (type 4). Examples are $Pmmm(00\gamma)$ (type 1), $Pmmm1'(00\gamma)$ (type 2), $Pmm'm'(00\gamma)$ (type 3) and $P_ammm(00\gamma)$ (type 4).

More generally, an incommensurate spin wave is given by

$$\mathbf{S}(\mathbf{r}) = \sum_{\mathbf{k}} \hat{\mathbf{S}}(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{r}). \tag{1.10.2.13}$$

This wave may be embedded in $n$-dimensional superspace as

$$\mathbf{S}(\mathbf{r}, \mathbf{r}_I) = \sum_{\mathbf{k}} \hat{\mathbf{S}}(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{r} + i\mathbf{k}_I \cdot \mathbf{r}_I). \tag{1.10.2.14}$$

The action of a superspace-group element $g = (g_E, g_I)$ then is given by

$$T_g\mathbf{S}(\mathbf{r}, \mathbf{r}_I) = \mathrm{Det}(R_E) R_E \mathbf{S}(g_E^{-1}\mathbf{r}, g_I^{-1}\mathbf{r}_I) \tag{1.10.2.15}$$

and the action of a superspace-group element $g$ with time reversal $\theta$ by

$$T_g\theta\mathbf{S}(\mathbf{r}, \mathbf{r}_I) = -\mathrm{Det}(R_E) R_E \mathbf{S}(g_E^{-1}\mathbf{r}, g_I^{-1}\mathbf{r}_I). \tag{1.10.2.16}$$

The action of the magnetic superspace group on the modulation function $\mathbf{u}(\mathbf{r}, \mathbf{r}_I)$ is given by the analogous expression

$$T_g\mathbf{u}(\mathbf{r}, \mathbf{r}_I) = R_E \mathbf{u}(g_E^{-1}\mathbf{r}, g_I^{-1}\mathbf{r}_I) \tag{1.10.2.17}$$

and the operator $\theta$ leaves the modulation function invariant. The magnetic superspace group then is the group of all elements $(g_E, g_I)$ and $(g_E, g_I)\theta$ leaving the spin wave and its nuclear structure in superspace invariant. The nuclear structure is invariant under time reversal. Magnetic superspace groups were introduced in Janner & Janssen (1980) and applied in, for example, Schobinger-Papamantellos *et al.* (1993) and Perez-Mato *et al.* (2012).

Equations (1.10.2.15)–(1.10.2.17) determine the (magnetic) superspace group if the nuclear and magnetic structures are known. Of course, if one assumes a certain magnetic superspace group, these equations restrict the possible spin wave functions, and analogously for the modulation functions in the nuclear structure.

### 1.10.2.5. *Pseudotensors*

In three dimensions, a quantity with three components is called a vector if it transforms according to the irreducible $L = 1$ representation of the orthogonal group $O(3)$. Because a point group $K$ is a subgroup of $O(3)$, the $L = 1$ representation restricted to $K$ gives the vector representation of $K$, which is generally reducible. If a quantity with three components transforms according to the vector representation for the elements of $K$ with determinant +1, and gets an additional minus sign for the other elements, the quantity is a pseudovector (see Section 1.2.4.1). Analogous definitions hold for tensors and pseudotensors.

In principle, one could use this terminology for higher dimensions, in particular for the superspace. However, in superspace the physical and internal subspaces have a different character, and the simple extension of the definition from three to $n$ dimensions is not very useful. It makes more sense to distinguish physical vectors (vectors in $V_E$), internal vectors (vectors in $V_I$) and tensor spaces, being the tensor product of two (or more) physical vector spaces, two or more internal vector spaces and mixed types, the simplest being the product of a physical and an internal vector space. A physical vector field is a function defined on the superspace, with values in $V_E$. An example is a phonon displacement field. Analogously, an internal vector field is a function with values in $V_I$. An example is a phason displacement in the direction of internal space. An example of a physical pseudovector field is a spin wave. It has three physical components and depends on the position in superspace. However, it is a pseudovector field, because under an element of the superspace point group it gets an additional minus sign for elements of $K_E$

with determinant $-1$. In addition, it gets an additional minus sign under time reversal. Therefore, it is a pseudovector field under time reversal.

An example of a pseudotensor is the magnetoelectric tensor $M$. For electric and magnetic fields the bilinear term in the energy is given by

$$E = \sum_{ij} M_{ij} E_i H_j. \tag{1.10.2.18}$$

This is a pseudotensor under space inversion and time reversal. The tensor $M$ transforms as the product of the vector representation of the point group with itself and with the determinant representation (for the pseudovector character of $H$).

### 1.10.3. Action of the symmetry group

1.10.3.1. *Action of superspace groups*

The action of the symmetry group on the periodic density function $\rho_s$ in $n$ dimensions is given by (1.10.2.9). The real physical structure, however, lives in physical space. One can derive from the action of the superspace group on the periodic structure its action on the quasiperiodic $d$-dimensional one. One knows that the density function in $V_E$ is just the restriction of that in $V_s$. The same holds for the transformed function.

$$g\rho_s(\mathbf{r}_s) = \rho_s(g^{-1}\mathbf{r}_s) \rightarrow g\rho(\mathbf{r}) = \rho_s[R^{-1}(\mathbf{r} - \mathbf{a}_E), -R_I^{-1}\mathbf{a}_I]. \tag{1.10.3.1}$$

This transformation property differs from that under an $n$-dimensional Euclidean transformation by the 'phase shift' $-R_I^{-1}\mathbf{a}_I$. Take for example the IC phase with a sinusoidal modulation. If the positions of the atoms are given by

$$\mathbf{n} + \mathbf{r}_j + \mathbf{A}_j \cos(2\pi\mathbf{Q}\cdot\mathbf{n} + \varphi_j),$$

then the transformed positions are

$$R(\mathbf{n} + \mathbf{r}_j) + R\mathbf{A}_j \cos(2\pi\mathbf{Q}\cdot\mathbf{n} + \varphi_j - R_I^{-1}\mathbf{a}_I) + \mathbf{a}_E. \tag{1.10.3.2}$$

If the transformation $g$ is a symmetry operation, this means that the original and the transformed positions are the same.

$$R(\mathbf{n} + \mathbf{r}_j) + \mathbf{a}_E = \mathbf{n}' + \mathbf{r}_{j'}$$

and

$$R\mathbf{A}_j \cos(2\pi\mathbf{Q}\cdot\mathbf{n} + \varphi_j - R_I^{-1}\mathbf{a}_I) = \mathbf{A}_{j'} \cos(2\pi\mathbf{Q}\cdot\mathbf{n}' + \varphi_{j'}).$$

This puts, in general, restrictions on the modulation.

Another view of the same transformation property is given by Fourier transforming (1.10.2.9). The result for the Fourier transform is

$$g\hat{\rho}_s(\mathbf{k}_s) = \hat{\rho}_s(R_s^{-1}\mathbf{k}_s)\exp(-i\mathbf{k}_s\cdot\mathbf{a}_s) \tag{1.10.3.3}$$

and because there is a one-to-one correspondence between the vectors $\mathbf{k}_s$ in the reciprocal lattice and the vectors $\mathbf{k}$ in the Fourier module one can rewrite this as

$$g\hat{\rho}(\mathbf{k}) = \hat{\rho}(R^{-1}\mathbf{k})\exp(-i\mathbf{k}\cdot\mathbf{a}_E - \mathbf{k}_I\cdot\mathbf{a}_I). \tag{1.10.3.4}$$

For a symmetry element one has $g\hat{\rho}(\mathbf{k}) = \hat{\rho}(\mathbf{k})$. Therefore, the superspace group element $g$ is a symmetry transformation of the quasiperiodic function $\rho$ if

$$\hat{\rho}(\mathbf{k}) = \hat{\rho}(R^{-1}\mathbf{k})\exp(-i\mathbf{k}\cdot\mathbf{a}_E - \mathbf{k}_I\cdot\mathbf{a}_I). \tag{1.10.3.5}$$

This relation is at the basis of the *systematic extinctions*. If one has an orthogonal transformation $R$ such that this in combination with a translation $(\mathbf{a}_E, \mathbf{a}_I)$ is a symmetry element and such that $R\mathbf{k} = \mathbf{k}$, then

$$\hat{\rho}(\mathbf{k}) = 0 \text{ if } \mathbf{k}\cdot\mathbf{a}_E + \mathbf{k}_I\cdot\mathbf{a}_I \neq 2\pi \times \text{integer}. \tag{1.10.3.6}$$

Because the structure factor is the Fourier transform of a density function which consists of $\delta$ functions on the positions of the atoms, for a quasiperiodic crystal it is the Fourier transform of a quasiperiodic function $\rho(\mathbf{r})$. Therefore, symmetry-determined absence of Fourier components leads to zero intensity of the corresponding diffraction peaks. Therefore, although there is no lattice periodicity for aperiodic crystals, systematic extinctions follow in the same way from the symmetry as in lattice periodic systems if one considers the $n$-dimensional space group as the symmetry group.

1.10.3.2. *Compensating gauge transformations*

The transformation property of the Fourier transform of the density given in the previous section can be formulated in another way. Consider a function $\rho(\mathbf{r})$ which is invariant under a $d$-dimensional Euclidean transformation $\{R|\mathbf{a}\}$ in physical space. Then its Fourier transform satisfies

$$\hat{\rho}(\mathbf{k}) = \hat{\rho}(R^{-1}\mathbf{k})\exp(-i\mathbf{k}\cdot\mathbf{a}). \tag{1.10.3.7}$$

Conversely, if the Fourier transform satisfies this relation, the Euclidean transformation is a symmetry operation for $\rho(\mathbf{r})$. The two equations (1.10.3.5) and (1.10.3.7) are closely related. One can also write (1.10.3.5) as

$$\hat{\rho}(\mathbf{k}) = \hat{\rho}(R^{-1}\mathbf{k})\exp(-i\mathbf{k}\cdot\mathbf{a})\exp[i\Phi(R,\mathbf{k})], \tag{1.10.3.8}$$

where $\Phi(R,\mathbf{k})$ can be considered as a gauge transformation that compensates for the phase shift: it is a *compensating gauge transformation*. It is a function that is linear in $\mathbf{k}$,

$$\Phi(R,\mathbf{k}+\mathbf{k}') = \Phi(R,\mathbf{k}) + \Phi(R,\mathbf{k}') \text{ (mod } 2\pi), \tag{1.10.3.9}$$

and satisfies a relation closely related to the one satisfied by nonprimitive translations.

$$\Phi(R,\mathbf{k}) + \Phi(S, R\mathbf{k}) = \Phi(RS,\mathbf{k}) \text{ (mod } 2\pi). \tag{1.10.3.10}$$

[Recall that a system of nonprimitive translations $\mathbf{u}(R)$ satisfies $\mathbf{u}(R) + R\mathbf{u}(S) = \mathbf{u}(RS)$ modulo lattice translations.] Therefore, the Euclidean transformation $\{R|\mathbf{a}\}$ combined with the compensating gauge transformation with gauge function $\Phi(R,\mathbf{k})$ is a symmetry transformation for $\rho(\mathbf{r})$ if equation (1.10.3.8) is satisfied. This is a three-dimensional formulation of the superspace group symmetry relation (1.10.3.5).

1.10.3.3. *Irreducible representations of three-dimensional space groups*

A third way to describe the symmetry of a quasiperiodic function is by means of irreducible representations of a space group. For the theory of these representations we refer to Chapter 1.2 on representations of crystallographic groups.

Consider first a modulated IC phase. Suppose the positions of the atoms are given by

$$\mathbf{n} + \mathbf{r}_j + \mathbf{u}_{\mathbf{n}j}, \tag{1.10.3.11}$$

where $\mathbf{n}$ belongs to the lattice, $\mathbf{r}_j$ is a position inside the unit cell and $\mathbf{u}_{\mathbf{n}j}$ is a displacement. If the structure is quasiperiodic with Fourier module $M^*$, the vectors $\mathbf{u}_{\mathbf{n}j}$ can be written as a superposition of normal modes.

$$\mathbf{u}_{\mathbf{n}j} = \sum_{\mathbf{k}\in M^*,\nu} Q_{k\nu}\boldsymbol{\varepsilon}(\mathbf{k}\nu|j)\mathrm{e}^{i\mathbf{k}\cdot\mathbf{n}} + c.c., \tag{1.10.3.12}$$

where the coefficient $Q_{\mathbf{k}\nu}$ is a normal coordinate, $\nu$ denotes the band index and $\boldsymbol{\varepsilon}(\mathbf{k}\nu|j)$ denotes the polarization of the normal mode. The normal coordinates transform under a space group according to one of its irreducible representations. The relevant