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1.10. Tensors in quasiperiodic structures

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1.10.1. Quasiperiodic structures

1.10.1.1. *Introduction*

Many materials are known which show a well ordered state without lattice translation symmetry, often in a restricted temperature or composition range. This can be seen in the diffraction pattern from the appearance of sharp spots that cannot be labelled in the usual way with three integer indices. The widths of the peaks are comparable with those of perfect lattice periodic crystals, and this is a sign that the coherence length is comparable as well.

A typical example is K_2SeO_4, which has a normal lattice periodic structure above 128 K with space group *Pcmn*, but below this temperature shows satellites at positions $\gamma\mathbf{c}^*$, where γ is an irrational number, which in addition depends on temperature. These satellites cannot be labelled with integer indices with respect to the reciprocal basis $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ of the structure above the transition temperature. Therefore, the corresponding structure cannot be lattice periodic.

The diffraction pattern of K_2SeO_4 arises because the original lattice periodic *basic structure* is deformed below 128 K. The atoms are displaced from their positions in the basic structure such that the displacement itself is again periodic, but with a period that is *incommensurate* with respect to the lattice of the basic structure.

Such a *modulated structure* is just a special case of a more general type of structure. These structures are characterized by the fact that the diffraction pattern has sharp Bragg peaks at positions $\mathbf{H}$ that are linear combinations of a finite number of basic vectors:

$$\mathbf{H} = \sum_{i=1}^{n} h_i \mathbf{a}_i^* \quad (\text{integer } h_i). \tag{1.10.1.1}$$

Structures that have this property are called *quasiperiodic*. The minimal number n of basis vectors such that all h_i are integers is called the *rank* of the structure. If the rank is three and the vectors $\mathbf{a}_i$ do not all fall on a line or in a plane, the structure is just lattice periodic. Lattice periodic structures form special cases of quasiperiodic structures. The collection of vectors $\mathbf{H}$ forms the *Fourier module* of the structure. For rank three, this is just the *reciprocal lattice* of the lattice periodic structure.

The definition given above results in some important practical difficulties. In the first place, it is not possible to show experimentally that a wavevector has irrational components instead of rational ones, because an irrational number can be approximated by a rational number arbitrarily well. Very often the wavevector of the satellite changes with temperature. It has been reported that in some compounds the variation shows plateaux, but even when the change seems to be continuous and smooth one can not be sure about the irrationality. On the other hand, if the wavevector jumps from one rational position to another, the structure would always be lattice periodic, but the unit cell of this structure would vary wildly with temperature. This means that, if one wishes to describe the incommensurate phases in a unified fashion, it is more convenient to treat the wavevector as generically irrational. This experimental situation is by no means dramatic. It is similar to the way in which one can never be sure that the angles between the basis vectors of an orthorhombic lattice are really 90°, although this is a concept that no-one has problems understanding.

A second problem stems from the fact that the wavevectors of the Fourier module are dense. For example, in the case of K_2SeO_4 the linear combinations of $\mathbf{c}^*$ and $\gamma\mathbf{c}^*$ cover the c axis uniformly. To pick out a basis here could be problematic, but the intensity of the spots is usually such that choosing a basis is not a problem. In fact, one only observes peaks with an intensity above a certain threshold, and these form a discrete set. At most, the occurrence of scale symmetry may make the choice less obvious.

1.10.1.2. *Types of quasiperiodic crystals*

One may distinguish various families of quasiperiodic systems. [Sometimes these are also called incommensurate systems (Janssen & Janner, 1987).] It is not a strict classification, because one may have intermediate cases belonging to more than one family as well. Here we shall consider a number of pure cases.

An *incommensurately modulated structure* or *incommensurate crystal* (*IC*) phase is a periodically modified structure that without the modification would be lattice periodic. Hence there is a *basic structure* with space-group symmetry. The periodicity of the modification should be incommensurate with respect to the basic structure. The position of the jth atom in the unit cell with origin at the lattice point $\mathbf{n}$ is $\mathbf{n} + \mathbf{r}_j$ ($j = 1, 2, \ldots, s$).

For a *displacive modulation*, the positions of the atoms are shifted from a lattice periodic basic structure. A simple example is a structure that can be derived from the positions of the basic structure with a simple displacement wave. The positions of the atoms in the IC phase are then

$$\mathbf{n} + \mathbf{r}_j + \mathbf{f}_j(\mathbf{Q}\cdot\mathbf{n}) \quad [\mathbf{f}_j(x) = \mathbf{f}_j(x+1)]. \tag{1.10.1.2}$$

Here the *modulation wavevector* $\mathbf{Q}$ has irrational components with respect to the reciprocal lattice of the basic structure. One has

$$\mathbf{Q} = \alpha\mathbf{a}^* + \beta\mathbf{b}^* + \gamma\mathbf{c}^*, \tag{1.10.1.3}$$

where at least one of α, β or γ is irrational. A simple example is the function $\mathbf{f}_j(x) = \mathbf{A}_j\cos(2\pi x + \varphi_j)$, where $\mathbf{A}_j$ is the *polarization vector* and φ_j is the phase of the modulation. The diffraction pattern of the structure (1.10.1.2) shows spots at positions

$$\mathbf{H} = h_1\mathbf{a}^* + h_2\mathbf{b}^* + h_3\mathbf{c}^* + h_4\mathbf{Q}. \tag{1.10.1.4}$$

Therefore, the rank is four and $\mathbf{a}_4^* = \mathbf{Q}$. In a more general situation, the components of the atom positions in the IC phase are given by

$$\mathbf{n}^\alpha + \mathbf{r}_j^\alpha + \sum_m \mathbf{A}_j^\alpha(\mathbf{Q}_m)\cos(2\pi\mathbf{Q}_m\cdot\mathbf{n} + \varphi_{jm\alpha}), \quad \alpha = x, y, z. \tag{1.10.1.5}$$

Here the vectors $\mathbf{Q}_m$ belong to the Fourier module of the structure. Then there are vectors $\mathbf{Q}_j$ such that any spot in the diffraction pattern can be written as

$$\mathbf{H} = \sum_{i=1}^{3} h_i\mathbf{a}_i^* + \sum_{j=1}^{d} h_{3+j}\mathbf{Q}_j \tag{1.10.1.6}$$

and the rank is $3 + d$. The peaks corresponding to the basic structure [the combinations of the three reciprocal-lattice vectors

$\mathbf{a}_i^*$ $(i = 1, 2, 3)$] are called the *main reflections*, the other peaks are *satellites*. For the latter, at least one of the $h_4, \ldots, h_n$ is different from zero.

A second type of modulation is the *occupation* or *composition* modulation. Here the structure can again be described on the basis of a basic structure with space-group symmetry. The basic structure positions are occupied with a certain probability by different atom species, or by molecules in different orientations. In CuAu(II), the two lattice positions in a b.c.c. structure are occupied by either Cu and Au or by Au and Cu with a certain probability. This probability function is periodic in one direction with a period that is not a multiple of the lattice constant. In $NaNO_2$, the NO_2 molecules are situated at the centre of the orthorhombic unit cell. There are two possible orientations for the V-shaped molecule, and the probability for one of the orientations is a periodic function with periodicity along the a axis. In this case, the modulation wavevector $\alpha\mathbf{a}^*$ has a component α that strongly depends on temperature in a very narrow temperature range.

If the probability of finding species A in position $\mathbf{n} + \mathbf{r}_j$ or of finding one orientation of a molecule in that point is given by $P_j(\mathbf{Q} \cdot \mathbf{n})$, the probability for species B or the other orientation is of course $1 - P_j(\mathbf{Q} \cdot \mathbf{n})$. In the diffraction pattern, the spots belong to the Fourier module with basic vectors $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ and $\mathbf{Q}$. The analogous expression for a more general situation with more modulation wavevectors, or with more species or orientations, is a straightforward generalization.

The first examples of IC phases were found in *magnetic systems* (see Section 1.5.1.2.3). For example, holmium has a spiral spin arrangement with a periodicity of the spiral that does not fit with the underlying lattice. For the α component $(\alpha = x, y, z)$ of the magnetic moment at position $\mathbf{n} + \mathbf{r}_j$ one has in an incommensurate magnetic system a superposition of waves

$$S_\alpha(\mathbf{n}j) = \sum_m M_{m\alpha j} \cos(2\pi \mathbf{Q}_m \cdot \mathbf{n} + \varphi_{m\alpha}). \tag{1.10.1.7}$$

The most general expression is

$$S_\alpha(\mathbf{n}j) = \sum_{\mathbf{H} \in M^*} M_{\alpha j}(\mathbf{H}) \exp(i\mathbf{H} \cdot \mathbf{n}), \tag{1.10.1.8}$$

where M^* is the Fourier module (1.10.1.1).

A following class of quasiperiodic materials is formed by *incommensurate composite structures*. To this belong misfit structures, intercalates and incommensurate adsorbed layers. An example is $Hg_{3-x}AsF_6$. This consists of a subsystem of AsF_6 octahedra forming a (modulated) tetragonal system and two other subsystems consisting of Hg chains, one system of chains in the x direction and one in the y direction. Because the average spacing between the Hg atoms is irrational with respect to the lattice constant of the host AsF_6 system in the same direction, the total structure does not have lattice periodicity in the a or b direction.

In general, there are two or more subsystems, labelled by ν, and the atomic positions are given by

$$\mathbf{n}_\nu + \mathbf{r}_{\nu j} + \text{modulation}, \tag{1.10.1.9}$$

where $\mathbf{n}_\nu$ belongs to the νth lattice, and where the modulation is a quasiperiodic displacement from the basic structure. The diffraction pattern has wavevectors

$$\mathbf{H} = \sum_\nu \sum_{i_\nu=1}^{3} h_{i_\nu} \mathbf{a}_{\nu i_\nu}^* = \sum_{i=1}^{n} h_i \mathbf{a}_i. \tag{1.10.1.10}$$

Each of the reciprocal-lattice vectors $\mathbf{a}_{\nu j}^*$ belongs to the Fourier module M^* and can be expressed as a linear combination with integer coefficients of the n basis vectors $\mathbf{a}_i^*$.

Very often, composite structures consist of a host system in the channels of which another material diffuses with a different, and incommensurate, lattice constant. Examples are layer systems in which foreign atoms intercalate. Another type of structure that belongs to this class is formed by adsorbed monolayers, for example a noble gas on a substrate of graphite. If the natural lattice constant of the adsorbed material is incommensurate with the lattice constant of the substrate, the layer as a whole will be quasiperiodic.

In general, the subsystems can not exist as such. They form idealized lattice periodic structures. Because of the interaction between the subsystems the latter will, generally, become modulated, and even incommensurately modulated because of the mutual incommensurability of the subsystems. The displacive modulation will, generally, contain wavevectors that belong to the Fourier module (1.10.1.10). However, in principle, additional satellites may occur due to other mechanisms, and this increases the rank of the Fourier module.

The last class to be discussed here is that of *quasicrystals*. In 1984 it was found (Shechtman *et al.*, 1984) that in the diffraction pattern of a rapidly cooled AlMn alloy the spots were relatively sharp and the point-group symmetry was that of an icosahedron, a group with 120 elements and one that can not occur as point group of a three-dimensional space group. Later, ternary alloys were found with the same symmetry of the diffraction pattern, but with spots as sharp as those in ordinary crystals. These structures were called quasicrystals. Others have been found with eight-, ten- or 12-fold rotation symmetry of the diffraction pattern. Such symmetries are also *noncrystallographic symmetries* in three dimensions. Sometimes this noncrystallographic symmetry is considered as characteristic of quasicrystals.

Mathematical models for quasicrystals are quasiperiodic *two- and three-dimensional tilings*, plane or space coverings, without voids or overlaps, by copies of a finite number of 'tiles'. Examples are the Penrose tiling or the standard octagonal tiling in two dimensions, and a three-dimensional version of Penrose tiling, a quasiperiodic space filling by means of two types of rhombohedra. For Penrose tiling, all spots of the diffraction pattern are linear combinations of the five basis vectors

$$\mathbf{a}_m^* = \{a\cos[2\pi(m-1)/5], a\sin[2\pi(m-1)/5]\} \quad (m = 1, \ldots 5). \tag{1.10.1.11}$$

Because the sum of these five vectors is zero, the rank of the spanned Fourier module is four. The Fourier module of the standard octagonal tiling is spanned by

$$\mathbf{a}_m^* = \{a\cos[(m-1)\pi/4], a\sin[(m-1)\pi/4]\} \quad (m = 1, \ldots, 4). \tag{1.10.1.12}$$

The rank of the Fourier module is four. The rank of the Fourier module of the three-dimensional Penrose tiling, consisting of two types of rhombohedra with a ratio of volumes of $(\sqrt{5}+1)/2$, is six and basis vectors point to the faces of a regular dodecahedron.

An atomic model can be obtained by decorating the tiles with atoms, each type of tile in a specific way. Some quasicrystals can really be considered as decorated tilings.

1.10.1.3. *Embedding in superspace*

A simple example of a quasiperiodic function is obtained in the following way. Consider a function of n variables which is periodic with period one in each variable.

$$f(x_1, \ldots, x_n) = f(x_1 + 1, x_2, \ldots, x_n), \ldots. \tag{1.10.1.13}$$

Now take n mutually irrational numbers α_i and define the function $g(x)$ with one variable as

$$g(x) = f(\alpha_1 x, \alpha_2 x, \ldots, \alpha_n x). \tag{1.10.1.14}$$

Because of the irrationality, the function $g(x)$ is not periodic. If we consider the Fourier transform of $f(x_1, \ldots, x_n)$ we get

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

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 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 Σ 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 Σ^*. 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 ρ_s to physical space is exactly ρ. Moreover, the function ρ_s is lattice periodic with lattice Σ, for which Σ^* 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 Σ^* with basis vectors $\mathbf{a}^*_{si}$ $(i = 1, 2, \ldots, n)$. The reciprocal lattice Σ^* corresponds to the direct lattice Σ. 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 Σ, 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 Σ, 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 ρ determines the function ρ_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*.

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 Σ^* invariant. Moreover, this transformation leaves the direct lattice Σ invariant as well. As always, the action of R_s on the basis of Σ 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 Σ 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

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

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 Σ 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 Σ^* 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

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

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

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

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

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 Σ^* 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

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

This group is an n-dimensional space group G. It has an invariant subgroup of translations, which is formed by the lattice translations Σ, and the quotient G/Σ 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

$$\{R_{s1}|\mathbf{a}_{s1}\}\{R_{s2}|\mathbf{a}_{s2}\} = \{R_{s1}R_{s2}|\mathbf{a}_{s1} + R_{s1}\mathbf{a}_{s2}\}. \tag{1.10.2.10}$$

On a lattice basis for Σ, 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 π, 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* (1999). 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).

1.10.3. Action of the symmetry group

1.10.3.1. *Action of superspace groups*

The action of the symmetry group on the periodic density function ρ_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 ρ 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 δ 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).

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, $\overline{10}$, $\bar{5}$
C_{12}	12	12, $\overline{12}$
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, $\overline{10}\,2m$, $\bar{5}m$
D_{12}	24	12 22, 12 mm, $\overline{12}\,2m$
$C_4 \times C_2$	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	$\bar{5}\bar{3}m$

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.

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

where the coefficient $Q_{\mathbf{k}\nu}$ is a normal coordinate, ν 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 space group here is that of the basic structure. For the simple case of a one-dimensional irreducible representation, for each $\mathbf{k}$ the effect is simply multiplication by a factor of absolute value unity. For example, for the modulated phase with basic space group *Pcmn* and wavevector $\mathbf{k} = \gamma\mathbf{c}^*$ there are four non-equivalent one-dimensional representations. It depends on the band index which representation occurs in the decomposition. The space-group element $\{R|\mathbf{a}\}$, for which $R\mathbf{q} = \mathbf{q}$ (modulo reciprocal lattice) acts on $Q_{\mathbf{k}\nu}$ according to

$$Q_{\mathbf{k}\nu} \rightarrow Q_{\mathbf{k}\nu}\exp(i\mathbf{k}.\cdot\mathbf{a})\chi_\nu(R),$$

where $\chi_\nu(R)$ is the character of R in an irreducible representation associated with the branch ν. Because the character of a one-dimensional representation is of absolute value unity, one may write it as $\exp[i\varphi_\nu(R,\mathbf{k})]$. Consequently, if the decomposition of the displacement contains only the vectors $\pm\mathbf{k}$, the factor $\exp[i\varphi_\nu(R,\mathbf{k})]$ describes a shift in the modulation function.

Consider again as an example a basic structure with space group *Pcmn* and a modulation wavevector $\gamma\mathbf{c}^*$. The point group $K_{\mathbf{k}}$ that leaves the modulation wavevector invariant is generated by m_y and m_x. This point group *mm*2 has four elements and four irreducible representations, all one-dimensional. One of them has for the character $\chi(m_x) = +1$, $\chi(m_y) = -1$. If the displacements of the atoms are described by a normal mode belonging to this irreducible representation, then the compensating phase shifts for c_x and m_y are, respectively, 0 and π. In the notation for superspace groups, this is the group $Pcmn(00\gamma)1s\bar{1}$. The same structure can be described by the irreducible representation characterized as Δ_3, because the modulation wavevector is the point Δ in the Brillouin zone and the irreducible representation Γ_3 has the character mentioned above.

In this way there is a correspondence between superspace groups for $(3+1)$-dimensional modulated structures and two-dimensional irreducible representations of three-dimensional space groups.

1.10.4. Tensors

1.10.4.1. *Tensors in higher-dimensional spaces*

A vector in an n-dimensional space V transforms under an element of a point group as $\mathbf{r} \rightarrow R\mathbf{r}$. With respect to a basis $\mathbf{a}_i$, the coordinates and basis vectors transform according to

$$\mathbf{a}'_i = \sum_{j=1}^{n} R_{ji}\mathbf{a}_j$$

$$\mathbf{r} = \sum_{i=1}^{n} x_i\mathbf{a}_i \rightarrow \mathbf{r}' = \sum_{i=1}^{n} x'_i\mathbf{a}_i, \quad x'_i = \sum_{j=1}^{n} R_{ij}x_j$$

and the reciprocal basis vectors and coordinates in reciprocal space according to

$$\mathbf{a}^*_i = \sum_{j=1}^{n} R_{ij}\mathbf{a}^{*'}_j$$

$$\mathbf{k} = \sum_{i=1}^{n} \kappa_i\mathbf{a}^*_i \rightarrow \mathbf{k}' = \sum_{i=1}^{n} \kappa'_i\mathbf{a}^*_i, \quad \kappa'_i = \sum_{j=1}^{n} R^{-1}_{ji}\kappa_j.$$

With respect to an orthonormal basis in V the transformations are represented by orthogonal matrices. For orthogonal matrices $R^{-1} = R^T$, the vectors in reciprocal space transform in exactly the same way as in direct space:

$$\mathbf{r} = \sum_{i=1}^{n} x_i\mathbf{e}_i \rightarrow \mathbf{r}' = \sum_{i=1}^{n} x'_i\mathbf{e}_i \quad x'_i = \sum_{i=1}^{n} R_{ij}x_i$$

$$\mathbf{k} = \sum_{i=1}^{n} \kappa_i\mathbf{e}^*_i \rightarrow \mathbf{k}' = \sum_{i=1}^{n} \kappa'_i\mathbf{e}^*_i \quad \kappa'_i = \sum_{i=1}^{n} R_{ij}\kappa_j.$$

As discussed in Section 1.2.4, a tensor is a multilinear function of vectors and reciprocal vectors. Consider for example a tensor of rank two, the metric tensor g. It is a function of two vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ which results in the scalar product of the two.

$$g(\mathbf{r}_1, \mathbf{r}_2) = \mathbf{r}_1 \cdot \mathbf{r}_2.$$

It clearly is a symmetric function because $g(\mathbf{r}_1, \mathbf{r}_2) = g(\mathbf{r}_2, \mathbf{r}_1)$. It is a function that is linear in each of its arguments and therefore

$$g(\mathbf{r}_1, \mathbf{r}_2) = g\left(\sum_{i=1}^{n} x_i\mathbf{e}_i, \sum_{j=1}^{n} y_j\mathbf{e}_j\right) = \sum_{ij} x_iy_j\delta_{ij} = \sum_{i} x_iy_j$$

if x_i and y_j are Cartesian coordinates of $\mathbf{r}_1$ and $\mathbf{r}_2$, respectively. For another basis, for example a lattice basis, one has coordinates ξ_i and η_j, and the same function becomes

$$g(\mathbf{r}_1, \mathbf{r}_2) = g\left(\sum_{i=1}^{n} \xi_i\mathbf{a}_i, \sum_{j=1}^{n} \eta_j\mathbf{a}_j\right) = \sum_{ij} \xi_i\eta_jg_{ij} \qquad (1.10.4.1)$$

with $g_{ij} = g(\mathbf{a}_i, \mathbf{a}_j)$. The relation between the Cartesian tensor components and the lattice tensor components follows from the basis transformation from orthonormal to a lattice basis. If

$$\mathbf{a}_j = \sum_{k} S_{kj}\mathbf{e}_k, \qquad (1.10.4.2)$$

then the lattice tensor components are

$$g_{ij} = \sum_{k} S_{ki}S_{kj}.$$

For example, in the two-dimensional plane a lattice spanned by $a(1,0)$ and $a(-\frac{1}{2}, \frac{1}{2}\sqrt{3})$ has a basis obtained from an orthonormal basis by the basis transformation

$$S = a\begin{pmatrix} 1 & -\frac{1}{2} \\ 0 & \frac{1}{2}\sqrt{3} \end{pmatrix}$$

and consequently the tensor components in lattice coordinates are

$$g_{ij} = \begin{pmatrix} a^2 & -\frac{1}{2}a^2 \\ -\frac{1}{2}a^2 & a^2 \end{pmatrix}.$$

The transformation of the tensor g under an orthogonal transformation follows from its definition. The transformation of the Cartesian tensor under the orthogonal transformation R is

$$g'_{ij} = \sum_{kl} R_{ki}R_{lj}g_{kl} = \sum_{kl} R_{ki}R_{lj}\delta_{kl} = \delta_{ij}$$

because of the fact that the matrix R_{ij} is orthogonal. The transformation of the tensor components with respect to the lattice basis, on which R is given by $\Gamma(R)$, is

$$g'_{ij} = \sum_{kl} \Gamma(R)_{ki}\Gamma(R)_{lj}g_{kl}, \qquad (1.10.4.3)$$

or in matrix form $g' = \Gamma(R)^T g\Gamma(R)$.

The metric tensor is invariant under a point group K if

$$g_{ij} = \sum_{kl} \Gamma(R)_{ki}\Gamma(R)_{lj}g_{kl} \quad \forall\ R \in K. \qquad (1.10.4.4)$$

On the one hand this formula can be used to determine the symmetry of a lattice with metric tensor g and on the other hand one may use it to determine the general form of a metric tensor invariant under a given point group. This comes down to the determination of the free parameters in g for given group of matrices $\Gamma(K)$. These are the coordinates in the space of invariant tensors.

1.10.4.2. *Tensors in superspace*

The tensors occurring for quasiperiodic structures are defined in a higher-dimensional space, but this space contains as privileged subspace the physical space. Since physical properties are measured in this physical space, the coordinates are not all on the same footing. This implies that sometimes one has to make a distinction between the various tensor elements as well.

The distinction between physical and internal (or perpendicular) coordinates can be made explicit by using a *split basis*. This is a basis for the superspace such that the first d basis vectors span the physical subspace and the other $n-d$ basis vectors the internal space. A lattice basis is, generally, not a split basis.

Let us consider again the metric tensor which is used to characterize higher-dimensional lattices as well, and in particular those corresponding to quasiperiodic structures. The elements $g_{ij} = g(\mathbf{a}_i, \mathbf{a}_j)$ transform according to

$$g'_{ij} = g(\mathbf{a}'_i, \mathbf{a}'_j) = \sum_{kl} R_{ki} R_{lj} g_{kl}.$$

The symmetry of an n-dimensional lattice with metric tensor g is the group of nonsingular $n \times n$ integer matrices S satisfying

$$g = S^T g S, \tag{1.10.4.5}$$

where ^{T} means the transpose. For a lattice corresponding to a quasiperiodic structure, this group is reducible into a d- and an $(n-d)$-dimensional component, where d is the dimension of physical space. This means that the d-dimensional component, which forms a finite group, is equivalent with a d-dimensional group of orthogonal transformations. In general, however, this does not leave a lattice in physical space invariant. However, it leaves the Fourier module of the quasiperiodic structure invariant. The basis vectors, for which the metric tensor determines the mutual relation, belong to the higher-dimensional superspace. Therefore, in this case the external and internal components of the basis vectors do not need to be treated differently. For the metric tensor g on a split basis one has

$$g_{ij} = 0 \quad \text{if} \quad i \le d, j > d \quad \text{or} \quad i > d, j \le d.$$

A quasiperiodic structure has an n-dimensional lattice embedding such that the intersection of Σ with the physical space V_E does not contain a d-dimensional lattice. Because of the incommensurability, however, there are lattice points of Σ arbitrarily close to V_E. This means that by an arbitrarily small shear deformation one may get a lattice in the physical space. The deformed quasiperiodic structure then becomes periodic. In general, the symmetry of the lattice then changes. This is certainly the case if the point group of the quasiperiodic structure is noncrystallographic, because then there cannot be a lattice in physical space left invariant by such a point group. For a given lattice Σ with symmetry group K one may ask which subgroups allow a deformation of the lattice that gives periodicity in V_E.

Physical tensors give often relations between vectorial or tensorial properties. Then they are multilinear functions of p vectors (and possibly q reciprocal vectors). An example is the dielectric tensor ε that gives the relation between E and D fields. This relation and the corresponding expression for the free energy F are

$$D_i = \sum_j \varepsilon_{ij} E_j \quad \text{or} \quad F = \sum_{ij} E_i \varepsilon_{ij} E_j = \varepsilon(\mathbf{E}, \mathbf{E}). \tag{1.10.4.6}$$

Therefore, the ε tensor is a bilinear function of vectors. The difference from the metric tensor is that here the vectors E and D are physical quantities which have d components and lie in physical space. The transformation properties therefore only depend on the physical-space components R_E of the superspace point group, and not on the full transformations R.

An intermediate case occurs for the strain. The strain tensor S gives the relation between a displacement and its origin: the point $\mathbf{r}$ is displaced to $\mathbf{r} + \Delta\mathbf{r}$ with $\Delta\mathbf{r}$ linear in $\mathbf{r}$:

$$\Delta\mathbf{r}_i = \sum_j S_{ij} \mathbf{r}_j.$$

In ordinary elasticity, both $\mathbf{r}$ and $\Delta\mathbf{r}$ belong to the physical space, and the relevant tensor is the symmetric part of S:

$$\tfrac{1}{2}(\partial_i \Delta\mathbf{r}_j + \partial_j \Delta\mathbf{r}_i).$$

For a quasiperiodic structure, $\Delta\mathbf{r}$ may be either a vector in physical space or in superspace and may depend both on physical and internal coordinates. That means that the matrix σ is either $d \times d$, or $n \times d$ or $n \times n$. Displacements in physical space are said to affect the *phonon degrees of freedom*, those in internal space the *phason degrees of freedom*. The phonon and phason displacements are functions of the physical-space coordinates. The transformation of the strain tensor under an element of a superspace group is

$$S'_{ij} = \sum_{k=1}^{d} \sum_{l=1}^{d} R_{Eki} R_{Elj} S_{kl} \text{ for phonon degrees,}$$

$$S'_{ij} = \sum_{k=d+1}^{n} \sum_{l=1}^{d} R_{lki} R_{Elj} S_{kl} \text{ for phason degrees,}$$

$$S'_{ij} = \sum_{k=1}^{n} \sum_{l=1}^{n} R_{ski} R_{slj} S_{kl} \text{ for the general case.}$$

The first two of these expressions apply only to a split basis, but the third can be written on a lattice basis.

$$\sum_{k,l=1}^{n} \Gamma(R)_{ki} \Gamma(R)_{lj} S_{kl}. \tag{1.10.4.7}$$

The tensor of elastic stiffnesses c gives the relation between stress T and strain S. The stress tensor is a physical tensor of rank two and dimension three. For the phonon strain one has

$$S_{ij} = \sum_{kl}^{3} c_{ijkl} T_{kl}, \quad (i, j = 1, \ldots, 3). \tag{1.10.4.8}$$

The phonon part of the elasticity tensor is symmetric under interchange of ij and kl, i and j, and k and l. It can be written in the usual notation $c_{\mu\nu}$ with $\mu, \nu = 1, 2, \ldots, 6$ with $1 = (11)$, $2 = (22)$, $3 = (33)$, $4 = (23)$, $5 = (13)$, $6 = (12)$. Its transformation property under a three-dimensional orthogonal transformation is

$$c'_{ijkl} = \sum_{i'j'k'l'} R_{i'i} R_{j'j} R_{k'k} R_{l'l} c_{i'j'k'l'}.$$

For the phason part a similar elasticity tensor is defined. This and the third elastic contribution, the coupling between phonons and phasons, will be discussed in Section 1.10.4.5.

1.10.4.3. *Inhomogeneous tensors*

A vector field in d-dimensional space assigns a vector to each point of the space. This vector-valued function may, for a quasi-

periodic system, have values in physical space or in superspace. In both cases one has the transformation property

$$g\mathbf{f}_i(\mathbf{r}) = \sum_j R_{ji}\mathbf{f}_j(g^{-1}\mathbf{r}). \qquad (1.10.4.9)$$

For a vector field in physical space, i and j run over the values $1, 2, 3$. This vector field may, however, be quasiperiodic. This means that it may be embedded in superspace. Then

$$g\mathbf{f}_i(\mathbf{r}_s) = \sum_{j=1}^{3} R_{Eji}\mathbf{f}_j\big[R_E^{-1}(\mathbf{r}-\mathbf{a}), R_I^{-1}(\mathbf{r}_I-\mathbf{a}_I)\big]. \qquad (1.10.4.10)$$

Here $i = 1, 2, 3$. If the vector field has values in superspace, as one can have for a displacement, one has

$$g\mathbf{f}_i(\mathbf{r}_s) = \sum_{j=1}^{n} R_{sji}\mathbf{f}_j\big[R_E^{-1}(\mathbf{r}-\mathbf{a}), R_I^{-1}(\mathbf{r}_I-\mathbf{a}_I)\big]. \qquad (1.10.4.11)$$

Here $i = 1, \ldots, n$. For Cartesian coordinates with respect to a split basis, R_s acts separately on physical and internal space and one has

$$g\mathbf{f}_i(\mathbf{r}_s) = \sum_{j=d+1}^{n} R_{Iji}\mathbf{f}_j\big[R_E^{-1}(\mathbf{r}-\mathbf{a}), R_I^{-1}(\mathbf{r}_I-\mathbf{a}_I)\big] \qquad (1.10.4.12)$$

for $i = d+1, \ldots, n$.

Just as for homogeneous tensors, inhomogeneous tensors may be divided into physical tensors with components in physical space only and others that have components with respect to an n-dimensional lattice. A physical tensor of rank two transforms under a space-group element $g = \{R_s|\mathbf{a}_s\}$ as

$$(gT)_{ij}(\mathbf{r}_s) = \sum_{k=1}^{d}\sum_{l=1}^{d} R_{Eki}R_{Elj}T_{kl}[R_E^{-1}(\mathbf{r}_E-\mathbf{a}_E), R_I^{-1}(\mathbf{r}_I-\mathbf{a}_I)]. \qquad (1.10.4.13)$$

This implies the following transformation property for the Fourier components:

$$(g\hat{T})_{ij}(\mathbf{k}) = \sum_{k=1}^{d}\sum_{l=1}^{d} R_{Eki}R_{Elj}T_{kl}(R_E^{-1}\mathbf{k})\exp(iR_E\mathbf{k}.\mathbf{a}_E + iR_I\mathbf{k}_I.\mathbf{a}_I). \qquad (1.10.4.14)$$

This gives relations between various Fourier components and restrictions for wavevectors $\mathbf{k}$ for which $R_E\mathbf{k} = \mathbf{k}$:

$$\hat{T}_{ij}(\mathbf{k}) = \sum_{k=1}^{d}\sum_{l=1}^{d} R_{Eki}R_{Elj}T_{kl}(\mathbf{k})\exp(iR_E\mathbf{k}.\mathbf{a}_E + iR_I\mathbf{k}_I.\mathbf{a}_I). \qquad (1.10.4.15)$$

For tensors with superspace components, the summation over the indices runs from 1 to n. An invariant tensor then satisfies

$$\hat{T}_{ij}(\mathbf{k}) = \sum_{k=1}^{n}\sum_{l=1}^{n} R_{ski}R_{slj}T_{kl}(\mathbf{k})\exp(iR_E\mathbf{k}.\mathbf{a}_E + iR_I\mathbf{k}_I.\mathbf{a}_I). \qquad (1.10.4.16)$$

The generalization to higher-rank tensors is straightforward.

1.10.4.4. *Irreducible representations*

For the characterization of vectors and tensors one needs the irreducible and vector representations of the point groups. If the point group is crystallographic in three dimensions, these can be found in Chapter 1.2. All point groups for IC phases or composite structures belong to this category. Exceptions are the point groups for quasicrystals. For the finite point groups for structures up to rank six these are given in Table 1.10.5.1. This table presents:

(1) The character tables for the point groups

$5, \bar{5}, 5m, 52, \bar{5}m$

$10, \overline{10}, 10/m, 10\,mm, 10\,22, \overline{10}\,2m, 10/mmm$

$8, \bar{8}, 8/m, 8mm, 822, \bar{8}2m, 8/mmm$

$12, \overline{12}, 12/m, 12\,mm, 12\,22, \overline{12}\,2m, 12/mmm$

$532, \bar{5}\bar{3}m.$

(2) Matrices for the generators in the irreducible representations of the groups

$$\bar{5}m, 10/mmm, 8/mmm, 12/mmm, \bar{5}\bar{3}m.$$

(3) The vector representations and some tensor representations for the groups in the systems

$$\bar{5}m, 10/mmm, 8/mmm, 12/mmm, \bar{5}\bar{3}m.$$

The character tables can be used to determine the number of independent tensor elements. This is the dimension of subspace of tensors transforming with the identity representation. Tensors transform according to (properly symmetrized or antisymmetrized) tensor products of vector representations. The number of times the identity representation occurs in the decomposition of the tensor product into irreducible components is equal to the number of independent tensor elements and can be calculated with the multiplicity formula. A number of examples are given in the following section.

1.10.4.5. *Determining the number of independent tensor elements*

1.10.4.5.1. *Piezoelectric tensor*

(See Sections 1.1.4.4.3 and 1.1.4.10.1.) The strain in a crystal is determined by its displacement field. For a quasiperiodic crystal, this displacement can have components in the physical space V_E as well as in the internal space V_I. The first implies a local displacement of the material, the latter corresponds to a local deformation because of the shift in the internal coordinate, which is, for example, the phase of a modulation wave or a phason jump for a quasicrystal. The displacement in the point $\mathbf{r}$ is $u = [u_E(\mathbf{r}), u_I(\mathbf{r})]$. Denote u_E by $\mathbf{v}$ and u_I by $\mathbf{w}$. The strain tensor then is given by $\partial_i v_j$ and by $\partial_i w_k$. Here i and j run from 1 to the physical dimension d, and k from 1 to the internal dimension $n-d$. The antisymmetric part of $\partial_i v_j$ corresponds to a global rotation, which does not lead to an energy change. Therefore, the relevant tensors are

$$e_{ij} = (\partial_i v_j + \partial_j v_i)/2, \quad f_{ik} = \partial_i w_k, \quad (i, j = 1, \ldots, d; k = 1, \ldots, n-d). \qquad (1.10.4.17)$$

Both the phonon part e and the phason part f may be coupled to an external electric field E. A linear coupling is given by the piezoelectric tensor p_{ijk}. The free energy is given by

$$F = \int \mathrm{d}r \left(\sum_{ijk} p^e_{ijk}e_{ij}E_k + \sum_{ijk} p^f_{ijk}f_{ij}E_k\right).$$

The tensor e transforms with the symmetrized square of the vector representation in physical space, the tensor f according to the product of the vector representations in physical and internal space. Then p^e and p^f transform according to the product of these two representations with the vector representation in physical space, because E is a physical vector.

As an example, consider the decagonal phase with point group $10\,mm(10^3\,mm)$. The physical space is three-dimensional and

Table 1.10.4.1. *Characters of the point group* $10\,mm(10^3\,mm)$ *for representations relevant for elasticity* $\tau = (\sqrt{5}-1)/2$.

	Classes					
	E	A	A^2	B	AB	
Representation	1	12	12	20	15	Reduction
Γ_E	3	$1+\tau$	$-\tau$	0	-1	Γ_2
Γ_I	3	$-\tau$	$1+\tau$	0	-1	Γ_3
Γ_E^2	9	$2+\tau$	$1-\tau$	0	1	
$\Gamma_E(g^2)$	3	$-\tau$	$1+\tau$	0	3	
$\Gamma_e = (\Gamma_E)_s^2$	6	1	1	0	2	$\Gamma_1+\Gamma_5$
Γ_e^2	36	1	1	0	4	
$\Gamma_e(g^2)$	6	1	1	0	6	
$(\Gamma_e)_s^2$	21	1	1	0	5	$2\Gamma_1+\Gamma_4+3\Gamma_5$
$\Gamma_f = \Gamma_E \times \Gamma_I$	9	-1	-1	0	1	$\Gamma_4+\Gamma_5$
$(\Gamma_f)_s^2$	45	0	0	0	5	$2\Gamma_1+\Gamma_2+\Gamma_3+3\Gamma_4+5\Gamma_5$
$\Gamma_e \times \Gamma_f$	54	-1	-1	0	2	$\Gamma_1+2\Gamma_2+2\Gamma_3+4\Gamma_4+5\Gamma_5$

carries a $(2+1)$-reducible representation ($\Gamma_1 \oplus \Gamma_5$), the internal space an irreducible two-dimensional representation (Γ_7). The symmetrized square of the first is six-dimensional, and the product of first and second is also six-dimensional. The products of these two with the three-dimensional vector representation in physical space are both 18-dimensional. The first contains the identity representation three times, the other does not contain the identity representation. This implies that the piezoelectric tensor has three independent tensor elements, all belonging to p^e. The tensor p^f is zero.

1.10.4.5.2. *Elasticity tensor*

(See Section 1.3.3.2.) As an example of a fourth-rank tensor, we consider the elasticity tensor. The lowest-order elastic energy is a bilinear expression in e and f:

$$F = \int \mathrm{d}\mathbf{r} \left(\tfrac{1}{2} \sum_{ijkl} c^E_{ijkl} e_{ij} e_{kl} + \tfrac{1}{2} \sum_{ijkl} c^I_{ijkl} f_{ij} f_{kl} + \sum_{ijkl} c^{EI}_{ijkl} e_{ij} f_{kl} \right). \tag{1.10.4.18}$$

The elastic free energy is a scalar function. The integrand must be invariant under the operations of the symmetry group. When $\Gamma_E(K)$ is the vector representation of K in the physical space (*i.e.* the vectors in V_E transform according to this representation) and $\Gamma_I(K)$ the vector representation in V_I, the tensor e_{ij} transforms according to the symmetrized square of Γ_E and the tensor f_{ij} transforms according to the product $\Gamma_E \otimes \Gamma_I$. Let us call these representations Γ_e and Γ_f, respectively. This implies that the term that is bilinear in e transforms according to the symmetrized square of Γ_e, that the term bilinear in f transforms according to the symmetrized square of Γ_f, and that the mixed term transforms according to $\Gamma_e \otimes \Gamma_f$. The number of elastic constants follows from their transformation properties. If $d = 3$ and $n = 3+p$, the number of constants c^E is 21, the number of constants c^I is $3p(3p+1)/2$ and the number of c^{IE} is $18p$. Therefore, without symmetry conditions, there are altogether $3(2+p)(7+3p)/2$ elastic constants. For arbitrary dimension d of the physical space and dimension n of the superspace this number is

$$d(d+1)(d^2+d+2)/8 + pd(pd+1)/2 + d^2(d+1)p/2 = d(2p+d+1)(2+d+d^2+2pd)/8.$$

The number of independent elastic constants is the number of independent coefficients in F, and this is given by the number of invariants, *i.e.* the number of times the identity representation occurs as irreducible component of, respectively, the symmetrized square of Γ_e, the symmetrized square of Γ_f, and of $\Gamma_e \otimes \Gamma_f$. The first number is the number of elastic constants in classical theory. The other elastic constants involve the phason degrees of freedom, which exist for quasiperiodic structures. The theory of the generalized elasticity theory for quasiperiodic crystals has been given by Bak (1985), Lubensky *et al.* (1985), Socolar *et al.* (1986) and Ding *et al.* (1993).

As an example, we consider an icosahedral quasicrystal. The symmetry group 532 has five classes, which are given in Table 1.10.5.1. The vector representation is Γ_2. It has character $\chi(R) = 3, 1+\tau, -\tau, 0, -1$. The character of its symmetrized square is $6, 1, 1, 0, 2$. Then the character of the representation with which the elasticity tensor transforms is $21, 1, 1, 0, 5$. This representation contains the trivial representation twice. Therefore, there are two free parameters (c_{1111} and c_{1122}) in the elasticity tensor for the phonon degrees of freedom.

For the phason degrees of freedom, the displacements transform with the representation Γ_3. In this case, the phason elasticity tensor transforms with the symmetrized square of the product of Γ_2 and Γ_3. Its character is $45, 0, 0, 0, 5$. This representation contains the identity representation twice. This implies that this tensor also has two free parameters.

Finally, the coupling term transforms with the product of the symmetrized square of Γ_2, Γ_2 and Γ_3. This representation has character $54, -1, -1, 0, 2$ and consequently contains the identity representation once. In total, the number of independent elastic constants is five for icosahedral tensors. The fact that we have only used the rotation subgroup 532, instead of the full group $\bar{5}\bar{3}m$, does not change this number. The additional central inversion makes the irreducible representations either even or odd. The elasticity tensors should be even, and there are exactly as many even irreducible representations as odd ones. This is shown in Table 1.10.4.1 (*cf.* Table. 1.10.5.1 for the character table of the group 532).

1.10.4.5.3. *Electric field gradient tensor*

As an example, we consider a symmetric rank-two tensor, *e.g.* an electric field gradient tensor, in a system with superspace group symmetry $Pcmn(00\gamma)1s\bar{1}$. The Fourier transform of the tensor T_{ij} is nonzero only for multiples of the vector $\gamma\mathbf{c}^*$. The symmetry element consisting of a mirror operation M_y and a shift $\frac{1}{2}\mathbf{a}_{s4}$ in V_I then has

$$R_E\mathbf{k} = \mathbf{k}, \quad \mathbf{k}\cdot\mathbf{a}_E = 0, \quad R_I = +1, \quad \mathbf{k}_I \cdot \mathbf{a}_I = \pi.$$

Then equation (1.10.4.15) leads to the relation

$$\hat{T}(m\gamma\mathbf{c}^*) = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} = (-1)^m \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

with solution

$$\hat{T} = \begin{pmatrix} a_{11} & 0 & a_{13} \\ 0 & a_{22} & 0 \\ a_{13} & 0 & a_{33} \end{pmatrix} \quad (m \text{ even}),$$

$$\hat{T} = \begin{pmatrix} 0 & a_{12} & 0 \\ a_{12} & 0 & a_{23} \\ 0 & a_{23} & 0 \end{pmatrix} \quad (m \text{ odd}).$$

This symmetry of the tensor can, for example, be checked by NMR (van Beest *et al.*, 1983).

1.10.4.6. *Determining the independent tensor elements*

In the previous sections some physical tensors have been studied, for which in a number of cases the number of the independent tensor elements has been determined. In this section the problem of determining the invariant tensor elements themselves will be addressed.

Consider an orthogonal transformation R acting on the vector space V. Its action on basis vectors is given by

$$\mathbf{e}'_i = \sum_j R_{ji} \mathbf{e}_j. \tag{1.10.4.19}$$

If the basis is orthonormal, the matrix R_{ij} is orthogonal ($RR^T = E$). For a point group in superspace the action of R in V_E differs, in general, from that on V_I.

$$\mathbf{e}'_{Ei} = \sum_j R_{Eji} \mathbf{e}_{Ej}; \quad \mathbf{e}'_{Ii} = \sum_j R_{Iji} \mathbf{e}_{Ij}. \tag{1.10.4.20}$$

The action of R on the tensor product space $V_1 \otimes V_2$, with V_i either V_E or V_I, is given by

$$\mathbf{e}'_{1i} \otimes \mathbf{e}'_{2j} = \sum_k \sum_l R^1_{ki} R^2_{lj} \mathbf{e}_{1k} \otimes \mathbf{e}_{2l}. \tag{1.10.4.21}$$

If both R_i are orthogonal matrices, the tensor product is also orthogonal. For the symmetrized tensor square $(V \otimes V)_{\rm sym}$ the basis formed by $\mathbf{e}_i \otimes \mathbf{e}_i$ $(i = 1, \ldots)$ and $(\mathbf{e}_i \otimes \mathbf{e}_j + \mathbf{e}_j \otimes \mathbf{e}_i)/\sqrt{2}$ $(i < j)$ is orthogonal.

A vector $\sum_{ij} c_{ij} \mathbf{e}_i \otimes \mathbf{e}_j$ in the tensor product space is invariant if

$$RcR^T = c. \tag{1.10.4.22}$$

A tensor as a (possibly symmetric or antisymmetric) bilinear function with coefficients $f_{ij} = f(\mathbf{e}_i, \mathbf{e}_j)$ is invariant if the matrix f_{ij} satisfies

$$R^T f R = f. \tag{1.10.4.23}$$

For orthogonal bases the equations (1.10.4.22) and (1.10.4.23) are equivalent.

Which spaces have to be chosen for V_i depends on the physical tensor property. The algorithm for determining invariant tensors starts from the transformation of the basis vectors $\mathbf{e}_i$, from which the basis transformation in tensor space follows after due orthogonalization in the case of (anti)symmetric tensors. This procedure can be continued to obtain higher-rank tensors. For orthogonal bases the invariant subspace is spanned by vectors corresponding to the independent tensor elements. We give a number of examples below.

Table 1.10.4.2. *Sign change of $\partial_i E_j$ under the generators A, B, C*

	A	*B*	*C*
11	+	+	+
12	−	−	+
13	−	+	−
21	−	−	+
22	+	+	+
23	+	−	−
31	−	+	−
32	+	−	−
33	+	+	+
41	−	+	−
42	+	−	−
43	+	+	+

1.10.4.6.1. *Metric tensor for an octagonal three-dimensional quasicrystal*

From the Fourier module for an octagonal quasicrystal in 3D the generators of the point group can be expressed as 5D integer matrices. They are

$$A = 8(8^3) = \begin{pmatrix} 0 & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$B = m_z(1) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix}$$

and

$$C = m(m) = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

and span an integer representation of the point group $8/mmm(8^31mm)$. Solution of the three simultaneous equations $S^T g S = g$ is equivalent with the determination of the subspace of the 15D symmetric tensor space that is invariant under the point group. The space has as basis the elements e_{ij} with $i \leq j$. The solution is given by

$$g = \begin{pmatrix} g_{11} & g_{12} & 0 & -g_{12} & 0 \\ g_{12} & g_{11} & g_{12} & 0 & 0 \\ 0 & g_{12} & g_{11} & g_{12} & 0 \\ -g_{12} & 0 & g_{12} & g_{11} & 0 \\ 0 & 0 & 0 & 0 & g_{55} \end{pmatrix}.$$

If $\mathbf{e}_i \otimes \mathbf{e}_j$ is denoted by ij, the solution follows because 55 is left invariant by A, B and C, whereas the orbits of 11 and 12 are $11 \rightarrow 22 \rightarrow 33 \rightarrow 44 \rightarrow 11$ and $12 \rightarrow 23 \rightarrow 34 \rightarrow -14 \rightarrow 12$, respectively.

1.10.4.6.2. *EFG tensor for Pcmn*

The electric field gradient tensor transforms as the product of a reciprocal vector and a vector. In Cartesian coordinates the transformation properties are the same. The point group for the basic structure of many IC phases of the family of A_2BX_4 compounds is *mmm*, and the point group for the modulated phase is the 4D group $mmm(11\bar{1})$, with generators

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

$$C = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

The tensor elements $\partial_i E_j$ being indicated by ij, the transformation under the generators gives a factor ± 1 as shown in Table 1.10.4.2.

From this, it follows that the four independent tensor elements are $\partial_1 E_1$, $\partial_2 E_2$, $\partial_3 E_3$ and the phason part $\partial_4 E_3$.

1.10.4.6.3. *Elasticity tensor for a two-dimensional octagonal quasicrystal*

The point group of the standard octagonal tiling is generated by the 2D orthogonal matrices

$$A = \begin{pmatrix} \sqrt{1/2} & -\sqrt{1/2} \\ \sqrt{1/2} & \sqrt{1/2} \end{pmatrix}, \quad B = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}.$$

In the tensor space one has the following transformations of the basis vectors; they are denoted by ij for $\mathbf{e}_i \otimes \mathbf{e}_j$:

$$\begin{aligned} 11 &\to \tfrac{1}{2}(11 + 12 + 21 + 22) \\ 12 &\to \tfrac{1}{2}(-11 + 12 - 21 + 22) \\ 21 &\to \tfrac{1}{2}(-11 - 12 + 21 + 22) \\ 22 &\to \tfrac{1}{2}(11 - 12 - 21 + 22). \end{aligned}$$

In the space spanned by $a = 11$, $b = \sqrt{1/2}(12 + 21)$ and $c = 22$, the eightfold rotation is represented by the matrix

$$S_E = \begin{pmatrix} \frac{1}{2} & -\sqrt{1/2} & \frac{1}{2} \\ \sqrt{1/2} & 0 & -\sqrt{1/2} \\ \frac{1}{2} & \sqrt{1/2} & \frac{1}{2} \end{pmatrix}.$$

In the six-dimensional space with basis aa, $\sqrt{1/2}(ab + ba)$, $\sqrt{1/2}(ac + ca)$, bb, $\sqrt{1/2}(bc + cb)$ and cc, the rotation gives the transformation

$$\begin{pmatrix} \frac{1}{4} & \frac{1}{2} & \sqrt{2}/4 & \frac{1}{2} & \frac{1}{2} & \frac{1}{4} \\ -\frac{1}{2} & -\frac{1}{2} & 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ \sqrt{2}/4 & 0 & \frac{1}{2} & -\sqrt{1/2} & 0 & \sqrt{2}/4 \\ \frac{1}{2} & 0 & -\sqrt{1/2} & 0 & 0 & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & 0 & 0 & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{4} & -\frac{1}{2} & \sqrt{2}/4 & \frac{1}{2} & -\frac{1}{2} & \frac{1}{4} \end{pmatrix}.$$

The vector $\mathbf{v}$ such that $\mathbf{S} \cdot \mathbf{v} = \mathbf{v}$ then is of the form

$$\mathbf{v} = (v_1, 0, (v_1 - v_4)\sqrt{2}, v_4, 0, v_1)^T.$$

This vector is also invariant under the mirror B. This means that there are two independent phonon elastic constants c^E_{1111} and c^E_{1212}, whereas the other tensor elements satisfy the relations

$$\begin{aligned} c^E_{1112} = c^E_{1222} = 0, \quad c^E_{2222} = c^E_{1111}, \\ c^E_{1122} = (c^E_{1111} + c^E_{1212})\sqrt{1/2}. \end{aligned}$$

The internal component of the eightfold rotation is A^3, that of the mirror B is B itself. The phason strain tensor transforms with the tensor product of external and internal components. This implies that the basis vectors, denoted by ij ($i = 1, 2$; $j = 3, 4$), transform under the eightfold rotation according to

$$\begin{aligned} 13 &\to (-13 + 14 - 23 + 24)/2 \\ 14 &\to (-13 - 14 - 23 - 24)/2 \\ 23 &\to (13 - 14 - 23 + 24)/2 \\ 24 &\to (13 + 14 - 23 - 24)/2. \end{aligned}$$

The symmetrized tensor square of this matrix gives the transformation in the space of phason–phason elasticity tensors, the direct product of the transformations in the 3D phonon strain space and the 4D phason strain space gives the transformation in the space of phonon-–phason elasticity tensors. The first matrix is given by

$$\frac{1}{16}\begin{pmatrix} 1 & \sqrt{2} & -\sqrt{2} & -\sqrt{2} & 1 & -\sqrt{2} & -\sqrt{2} & 1 & \sqrt{2} & 1 \\ -\sqrt{2} & 0 & 2 & 0 & \sqrt{2} & 0 & -2 & -\sqrt{2} & 0 & \sqrt{2} \\ \sqrt{2} & 2 & 0 & 0 & \sqrt{2} & 0 & 0 & -\sqrt{2} & -2 & -\sqrt{2} \\ -\sqrt{2} & 0 & 0 & 2 & \sqrt{2} & -2 & 0 & \sqrt{2} & 0 & -\sqrt{2} \\ 1 & -\sqrt{2} & -\sqrt{2} & \sqrt{2} & 1 & \sqrt{2} & -\sqrt{2} & 1 & -\sqrt{2} & 1 \\ -\sqrt{2} & 0 & 0 & -2 & \sqrt{2} & 2 & 0 & \sqrt{2} & 0 & -\sqrt{2} \\ \sqrt{2} & -2 & 0 & 0 & \sqrt{2} & 0 & 0 & -\sqrt{2} & 2 & -\sqrt{2} \\ 1 & \sqrt{2} & \sqrt{2} & \sqrt{2} & 1 & \sqrt{2} & \sqrt{2} & 1 & \sqrt{2} & 1 \\ -\sqrt{2} & 0 & -2 & 0 & \sqrt{2} & 0 & 2 & -\sqrt{2} & 0 & \sqrt{2} \\ 1 & -\sqrt{2} & \sqrt{2} & -\sqrt{2} & 1 & -\sqrt{2} & \sqrt{2} & 1 & -\sqrt{2} & 1 \end{pmatrix}.$$

Vectors invariant under this operation and the transformation corresponding to the mirror B correspond to invariant elasticity tensors. For the transformation B, all tensor elements with an odd number of indices 1 or 3 are zero. In the space of phason–phason tensors the general invariant vector is

$$(x_1, 0, 0, -x_6 + (x_5 - x_1)\sqrt{2}, x_5, x_6, 0, x_5, 0, x_1).$$

There are three independent elastic constants, $x_1 = c_{1313}$, $x_5 = c_{1414}$ and $x_6 = c_{1423}$. For the phonon–phason elastic constants the corresponding invariant vector is

$$(x, 0, 0, x, 0, x/\sqrt{2}, -x/\sqrt{2}, 0, -x, 0, 0, -x).$$

The independent elastic constant is $x = c_{1113} = c_{1124} = c_{1214}\sqrt{2} = -c_{1223}\sqrt{2} = -c_{2213} = -c_{2224}$.

1.10.4.6.4. *Piezoelectric tensor for a three-dimensional octagonal quasicrystal*

A quasicrystal with octagonal point group $8/mmm(8^31mm)$ will not show a piezoelectric effect because the point group contains the central inversion. We consider here the point group $8mm(8^3mm)$ which is a subgroup without central inversion. It is generated by the matrices

$$A = \begin{pmatrix} \alpha & -\alpha & 0 & 0 & 0 \\ \alpha & \alpha & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -\alpha & -\alpha \\ 0 & 0 & 0 & \alpha & -\alpha \end{pmatrix},$$

$$B = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

Here $\alpha = \sqrt{2}/2$. There are two components for the strain, a phonon component e and a phason component f. The phonon strain tensors form a 6D space, the phason strain tensors also a 6D space. The phonon strain space transforms with the symmetrized square of the physical parts of the operations, the phason strain space with the product of physical and internal parts. For the eightfold rotation the corresponding matrices are

$$S_e = \begin{pmatrix} \frac{1}{2} & -\alpha & 0 & \frac{1}{2} & 0 & 0 \\ \alpha & 0 & 0 & -\alpha & 0 & 0 \\ 0 & 0 & \alpha & 0 & -\alpha & 0 \\ \frac{1}{2} & \alpha & 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \alpha & 0 & \alpha & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

$$S_f = \begin{pmatrix} -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & 0 & 0 \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\alpha & -\alpha \\ 0 & 0 & 0 & 0 & \alpha & -\alpha \end{pmatrix}.$$

The action on the space of piezoelectric tensors is given, for the phonon and the phason part, by taking the product of these matrices with the physical part A_E. The invariant vectors under these matrices give the invariant tensors. If the second generator is taken into account, which requires that the number of indices 1 or 4 is even, this results in the independent tensor elements

$$x_3 = c_{113}, \quad x_{16} = c_{322}, \quad x_{18} = c_{333}$$

with relation $c_{223} = c_{113}$, whereas all other elements are zero for the coupling between the electric field and phonon strain. There is no nontrivial invariant vector in the second case. Therefore, all tensor elements for the coupling between the electric field and phason strain are zero.

1.10.4.6.5. *Elasticity tensor for an icosahedral quasicrystal*

The point group of an icosahedral quasicrystal is $532(5^2 32)$ with generators having components

$$A_E = \begin{pmatrix} 1 & \tau & -1-\tau \\ \tau & 1+\tau & 1 \\ 1+\tau & -1 & \tau \end{pmatrix}/2,$$

$$B_E = \begin{pmatrix} -\tau & 1+\tau & -1 \\ 1+\tau & 1 & \tau \\ 1 & -\tau & -1-\tau \end{pmatrix}/2$$

in physical space and components

$$A_I = \begin{pmatrix} -1 & \tau & -1-\tau \\ -\tau & \tau^{-1} & 1 \\ 1+\tau & 1 & -\tau \end{pmatrix}/2, \quad B_I = \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

in internal space (see Table 1.10.5.2). The phonon and phason strain tensors form a 6D, respectively 9D, vector space, in which the point group acts with matrices

$$S_e = \frac{1}{4}\begin{pmatrix} 1 & \tau\sqrt{2} & -\varphi\sqrt{2} & 1-\tau & -\sqrt{2} & 2+\tau \\ \tau\sqrt{2} & 2 & 0 & \sqrt{2} & -2 & -\varphi\sqrt{2} \\ \varphi\sqrt{2} & 0 & -2 & -\tau\sqrt{2} & 2 & -\sqrt{2} \\ 1-\tau & \sqrt{2} & \tau\sqrt{2} & 2+\tau & \varphi\sqrt{2} & 1 \\ \sqrt{2} & 2 & 2 & -\varphi\sqrt{2} & 0 & \tau\sqrt{2} \\ 2+\tau & -\varphi\sqrt{2} & \sqrt{2} & 1 & -\tau\sqrt{2} & 1-\tau \end{pmatrix},$$

$$S_f = \frac{1}{4}\begin{pmatrix} -\tau & \varphi & -1 & \tau-1 & 1 & -\tau & 1 & -2-\tau & \varphi \\ \varphi & 1 & \tau & 1 & \tau & 1-\tau & -2-\tau & -\varphi & -1 \\ 1 & -\tau & -\varphi & \tau & \tau-1 & -1 & -\varphi & 1 & 2+\tau \\ \tau-1 & 1 & -\tau & -1 & 2+\tau & -\varphi & -\tau & \varphi & -1 \\ 1 & \tau & 1-\tau & 2+\tau & \varphi & 1 & \varphi & 1 & \tau \\ \tau & \tau-1 & -1 & \varphi & -1 & -2-\tau & 1 & -\tau & -\varphi \\ -1 & 2+\tau & -\varphi & \tau & -\varphi & 1 & \tau-1 & 1 & -\tau \\ 2+\tau & \varphi & 1 & -\varphi & -1 & -\tau & 1 & \tau & 1-\tau \\ \varphi & -1 & -2-\tau & -1 & \tau & \varphi & \tau & \tau-1 & -1 \end{pmatrix}$$

and

$$T_e = \frac{1}{4}\begin{pmatrix} 1 & -\tau\sqrt{2} & \varphi\sqrt{2} & 1-\tau & -\sqrt{2} & 2+\tau \\ \tau\sqrt{2} & -2 & 0 & \sqrt{2} & -2 & -\varphi\sqrt{2} \\ -\varphi\sqrt{2} & 0 & -2 & \tau\sqrt{2} & -2 & \sqrt{2} \\ 1-\tau & -\sqrt{2} & -\tau\sqrt{2} & 2+\tau & \varphi\sqrt{2} & 1 \\ -\sqrt{2} & 2 & 2 & \varphi\sqrt{2} & 0 & -\tau\sqrt{2} \\ 2+\tau & \varphi\sqrt{2} & -\sqrt{2} & 1 & -\tau\sqrt{2} & 1-\tau \end{pmatrix},$$

$$T_f = \frac{1}{2}\begin{pmatrix} 0 & 0 & 1 & 0 & 0 & -\tau & 0 & 0 & \varphi \\ 1 & 0 & 0 & -\tau & 0 & 0 & \varphi & 0 & 0 \\ 0 & -1 & 0 & 0 & \tau & 0 & 0 & -\varphi & 0 \\ 0 & 0 & \tau & 0 & 0 & -\varphi & 0 & 0 & -1 \\ \tau & 0 & 0 & -\varphi & 0 & 0 & -1 & 0 & 0 \\ 0 & -\tau & 0 & 0 & \varphi & 0 & 0 & 1 & 0 \\ 0 & 0 & -\varphi & 0 & 0 & -1 & 0 & 0 & \tau \\ -\varphi & 0 & 0 & -1 & 0 & 0 & \tau & 0 & 0 \\ 0 & \varphi & 0 & 0 & 1 & 0 & 0 & -\tau & 0 \end{pmatrix}.$$

This implies that the phonon elasticity tensors form a 21D space, the phason elasticity tensors a 45D space and the phonon–phason coupling a 54D space. The invariant vectors under these orthogonal transformations correspond to invariant elastic tensors. Their coordinates are the elastic constants. For the given presentation of the point group, these are given in Table 1.10.4.3. The tensor elements are expressed in parameters x and y where there are two independent tensor elements. The tensor elements that are not given are zero or equal to that given by the permutation symmetry. If bases for the phonon and phason strain are introduced by

$$[1] = 11, [2] = 12, [3] = 13, [4] = 22, [5] = 23, [6] = 33$$

for the phonon part and

$$[1] = 14, [2] = 15, [3] = 16, [4] = 24, [5] = 25, [6] = 26,$$
$$[7] = 34, [8] = 35, [9] = 36$$

for the phason part, the elastic tensors may be given in matrix form as

$$c^{ee} = \begin{pmatrix} x+y & 0 & 0 & x & 0 & x \\ 0 & y & 0 & 0 & 0 & 0 \\ 0 & 0 & y & 0 & 0 & 0 \\ x & 0 & 0 & x+y & 0 & x \\ 0 & 0 & 0 & 0 & y & 0 \\ x & 0 & 0 & x & 0 & x+y \end{pmatrix},$$

$$c^{ff} = \begin{pmatrix} z & \tau^2 u & -\tau u & -\tau u & \tau u & -\tau u & -u & 0 & \tau u \\ \tau^2 u & z-2\tau u & u & \tau u & u & 0 & 0 & \tau^2 u & \tau u \\ -\tau u & u & z & -\tau u & 0 & -\tau^2 u & \tau u & \tau u & \tau u \\ -\tau u & \tau u & -\tau u & z & \tau u & u & -\tau^2 u & \tau u & 0 \\ \tau u & u & 0 & \tau u & z & -\tau^2 u & \tau u & -\tau u & -\tau u \\ -\tau u & 0 & -\tau^2 u & u & -\tau^2 u & z-2\tau u & 0 & -\tau u & u \\ -u & 0 & \tau u & -\tau^2 u & \tau u & 0 & z-2\tau u & -u & -\tau^2 u \\ 0 & \tau^2 u & \tau u & \tau u & -\tau u & -\tau u & -u & z & -\tau u \\ \tau u & \tau u & \tau u & 0 & -\tau u & u & -\tau^2 u & -\tau u & z \end{pmatrix},$$

$$c^{ef} = \begin{pmatrix} -v & -\tau v & -\tau^2 v & -\tau^3 v & \tau v & -\tau^2 v & v & -\tau v & -\tau^{-1} v \\ -\tau^3 v & \tau v & -\tau^2 v & \tau^2 v & v & \tau v & 0 & 0 & 0 \\ v & -\tau v & -\tau^{-1} v & 0 & 0 & 0 & -\tau v & -\tau^2 v & -\tau^3 v \\ \tau^{-1} v & v & \tau v & -\tau^2 v & v & -\tau v & -\tau^2 v & -\tau^3 v & \tau v \\ 0 & 0 & 0 & -\tau^2 v & \tau^3 v & \tau v & \tau v & -\tau^{-1} v & v \\ -\tau v & -\tau^2 v & -\tau^3 v & \tau v & -\tau^{-1} v & v & -\tau v & \tau^2 v & v \end{pmatrix}.$$

The parameters x, y, z, u, v are the five independent elastic constants.

1.10.5. Tables

In this section are presented the irreducible representations of point groups of quasiperiodic structures up to rank six that do not occur as three-dimensional crystallographic point groups.

Table 1.10.4.3. *Elastic constants for icosahedral quasicrystals*

Type	Free parameters	Relations
Phonon–phonon	2	$c_{1111} = c_{2222} = c_{3333} = x$ $c_{1122} = c_{1133} = c_{2233} = y$ $c_{1212} = c_{1313} = c_{2323} = x - y$
Phason–phason	2	$c_{1414} = c_{1616} = c_{2424} = c_{2525} = c_{3535} = c_{3636} = x$ $c_{1416} = c_{1424} = -c_{1425} = c_{1426} = -c_{1436} = y$ $c_{1524} = c_{1536} = -c_{1624} = c_{1634} = c_{1635} = -y$ $c_{1636} = c_{2425} = c_{2435} = c_{2534} = -c_{2535} = -y$ $c_{2536} = c_{2635} = c_{3536} = y$, $c_{1515} = c_{2626} = c_{3434} = x + 2y$ $c_{1415} = c_{1535} = -c_{1626} = -c_{2434} = -c_{2526} = -c_{3436} = y\tau$ $c_{1434} = -c_{11516} = -c_{1525} = -c_{2426} = -c_{2636} = c_{3435} = y/\tau$
Phonon–phason	1	$-c_{1114} = c_{1134} = c_{1225} = c_{2225} = c_{2336} = c_{3326} = c_{3336}$ $= -c_{1115}/\tau = c_{1125}/\tau = -c_{1135}\tau = c_{1215}\tau = c_{1226}\tau$ $= -c_{1334}\tau = -c_{2226}\tau = c_{2236}\tau = c_{2326}\tau = c_{2334}\tau$ $= -c_{3334}\tau = -c_{1116}\tau^2 = -c_{1126}\tau^2 = -c_{1216}\tau^2$ $= -c_{1335}\tau^2 = -c_{2224}\tau^2 = -c_{2234}\tau^2 = c_{3335}\tau^2$ $= -c_{1136}\tau = c_{1224}\tau = -c_{1316}\tau = -c_{2335}\tau$ $= -c_{1124}/\tau^3 = -c_{1336}/\tau^3 = c_{2235}/\tau^3 = c_{2325}/\tau^3$

Table 1.10.5.1. *Character tables of some point groups for quasicrystals*

(*a*) C_5 [$\omega = \exp(2\pi i/5)$].

C_5	ε	α	α^2	α^3	α^4
n	1	1	1	1	1
Order	1	5	5	5	5
Γ_1	1	1	1	1	1
Γ_2	1	ω	ω^2	ω^3	ω^4
Γ_3	1	ω^2	ω^4	ω	ω^3
Γ_4	1	ω^3	ω	ω^4	ω^2
Γ_5	1	ω^4	ω^3	ω^2	ω

	Generators	Vector representation	Perpendicular representation
5	$\alpha = C_{5z}$	$\Gamma_1 \oplus \Gamma_2 \oplus \Gamma_5$	$\Gamma_3 \oplus \Gamma_4$

(*b*) D_5 [$\tau = (\sqrt{5} - 1)/2$].

D_5	ε	α	α^2	β
n	1	2	2	5
Order	1	5	5	2
Γ_1	1	1	1	1
Γ_2	1	1	1	-1
Γ_3	2	τ	$-1-\tau$	0
Γ_4	2	$-1-\tau$	τ	0

	Generators	Vector representation	Perpendicular representation
52	$\alpha = C_{5z}$ $\beta = C_{2x}$	$\Gamma_2 \oplus \Gamma_3$	Γ_4
$5m$	$\alpha = C_{5z}$ $\beta = m_x$	$\Gamma_1 \oplus \Gamma_3$	Γ_4
$\bar{5}m$	$\sim 52 \times \mathbb{Z}_2$	$\Gamma_{1u} \oplus \Gamma_{3u}$	Γ_{4u}

(*c*) C_8 [$\omega = \exp(\pi i/4) = (1+i)/\sqrt{2}$].

C_8	ε	α	α^2	α^3	α^4	α^5	α^6	α^7
n	1	1	1	1	1	1	1	1
Order	1	8	4	8	2	8	6	8
Γ_1	1	1	1	1	1	1	1	1
Γ_2	1	ω	i	ω^3	-1	ω^5	$-i$	ω^7
Γ_3	1	i	-1	$-i$	1	i	-1	$-i$
Γ_4	1	ω^3	$-i$	ω	-1	ω^7	i	ω^5
Γ_5	1	-1	1	-1	1	-1	1	-1
Γ_6	1	ω^5	i	ω^7	-1	ω	$-i$	ω^3
Γ_7	1	$-i$	-1	i	1	$-i$	-1	i
Γ_8	1	ω^7	$-i$	ω^5	-1	ω^3	i	ω

	Generators	Vector representation	Perpendicular representation
$\frac{8}{\bar{8}}$	$\alpha = C_{8z}$ $\alpha = S_{8z}$	$\Gamma_1 \oplus \Gamma_2 \oplus \Gamma_8$ $\Gamma_4 \oplus \Gamma_5 \oplus \Gamma_6$	$\Gamma_4 \oplus \Gamma_6$ $\Gamma_2 \oplus \Gamma_8$
$8/m$	$\sim 8 \times \mathbb{Z}_2$	$\Gamma_{1u} \oplus \Gamma_{2u} \oplus \Gamma_{8u}$	$\Gamma_{4u} \oplus \Gamma_{6u}$

(*d*) D_8

D_8	ε	α	α^2	α^3	α^4	β	$\alpha\beta$
n	1	2	2	2	1	4	4
Order	1	8	4	8	2	2	2
Γ_1	1	1	1	1	1	1	1
Γ_2	1	1	1	1	1	-1	-1
Γ_3	1	-1	1	-1	1	1	-1
Γ_4	1	-1	1	-1	1	-1	1
Γ_5	2	$\sqrt{2}$	0	$-\sqrt{2}$	-2	0	0
Γ_6	2	0	-2	0	2	0	0
Γ_7	2	$-\sqrt{2}$	0	$\sqrt{2}$	-2	0	0

	Generators	Vector representation	Perpendicular representation
822	$\alpha = C_{8z}$ $\beta = C_{2x}$	$\Gamma_2 \oplus \Gamma_5$	Γ_7
$8mm$	$\alpha = C_{8z}$ $\beta = m_x$	$\Gamma_1 \oplus \Gamma_5$	Γ_7
$\bar{8}2m$	$\alpha = S_{8z}$ $\beta = C_{2x}$	$\Gamma_3 \oplus \Gamma_7$	Γ_5
$8/mmm$	$\sim 822 \times \mathbb{Z}_2$	$\Gamma_{2u} \oplus \Gamma_{5u}$	Γ_{7u}

(*e*) C_{10} [$\omega = exp(2\pi i/5)$].

C_{10}	ε	α^2	α^4	α^6	α^8
n	1	1	1	1	1
Order	1	5	5	5	5
Γ_1	1	1	1	1	1
Γ_2	1	ω	ω^2	ω^3	ω^4
Γ_3	1	ω^2	ω^4	ω	ω^3
Γ_4	1	ω^3	ω	ω^4	ω^2
Γ_5	1	ω^4	ω^3	ω^2	ω
Γ_6	1	1	1	1	1
Γ_7	1	ω	ω^2	ω^3	ω^4
Γ_8	1	ω^2	ω^4	ω	ω^3
Γ_9	1	ω^3	ω	ω^4	ω^2
Γ_{10}	1	ω^4	ω^3	ω^2	ω

C_{10}	α^5	α^7	α^9	α	α^3
n	1	1	1	1	1
Order	2	10	10	10	10
Γ_1	1	1	1	1	1
Γ_2	1	ω	ω^2	ω^3	ω^4
Γ_3	1	ω^2	ω^4	ω	ω^3
Γ_4	1	ω^3	ω	ω^4	ω^2
Γ_5	1	ω^4	ω^3	ω^2	ω
Γ_6	-1	-1	-1	-1	-1
Γ_7	-1	$-\omega$	$-\omega^2$	$-\omega^3$	$-\omega^4$
Γ_8	-1	$-\omega^2$	$-\omega^4$	$-\omega$	$-\omega^3$
Γ_9	-1	$-\omega^3$	$-\omega$	$-\omega^4$	$-\omega^2$
Γ_{10}	-1	$-\omega^4$	$-\omega^3$	$-\omega^2$	$-\omega$

Table 1.10.5.1 (*cont.*)

	Generators	Vector representation	Perpendicular representation
$\underline{10}$ $\bar{5}$ $\overline{10}$	$\alpha = C_{10z}$ $\alpha = S_{5z}$ $\alpha = S_{10z}$	$\Gamma_1 \oplus \Gamma_7 \oplus \Gamma_{10}$ $\Gamma_6 \oplus \Gamma_8 \oplus \Gamma_9$ $\Gamma_2 \oplus \Gamma_4 \oplus \Gamma_6$	$\Gamma_8 \oplus \Gamma_9$ $\Gamma_7 \oplus \Gamma_{10}$ $\Gamma_3 \oplus \Gamma_5$
$10/m$	$\sim 10 \times \mathbb{Z}_2$	$\Gamma_{1u} \oplus \Gamma_{7u} \oplus \Gamma_{10u}$	$\Gamma_{8u} \oplus \Gamma_{9u}$

(*f*) D_{10} [$\tau = (\sqrt{5}-1)/2$].

D_{10}	ε	α	α^2	α^3
n	1	2	2	2
Order	1	10	5	10
Γ_1	1	1	1	1
Γ_2	1	1	1	1
Γ_3	1	-1	1	-1
Γ_4	1	-1	1	-1
Γ_5	2	$1+\tau$	τ	$-\tau$
Γ_6	2	τ	$-1-\tau$	$-1-\tau$
Γ_7	2	$-\tau$	$-1-\tau$	$1+\tau$
Γ_8	2	$-1-\tau$	τ	τ

D_{10}	α^4	α^5	β	$\alpha\beta$
n	2	1	5	5
Order	5	2	2	2
Γ_1	1	1	1	1
Γ_2	1	1	-1	-1
Γ_3	1	-1	1	-1
Γ_4	1	-1	-1	1
Γ_5	$-1-\tau$	-2	0	0
Γ_6	τ	2	0	0
Γ_7	τ	-2	0	0
Γ_8	$-1-\tau$	2	0	0

	Generators	Vector representation	Perpendicular representation
$10\,22$	$\alpha = C_{10z}$ $\beta = C_{2x}$	$\Gamma_2 \oplus \Gamma_5$	Γ_7
$10\,mm$	$\alpha = C_{10z}$ $\beta = m_x$	$\Gamma_1 \oplus \Gamma_5$	Γ_7
$\overline{10}\,2m$	$\alpha = S_{10z}$ $\beta = C_{2x}$	$\Gamma_4 \oplus \Gamma_8$	Γ_6
$\bar{5}m$	$\alpha = S_{5z}$ $\beta = C_{2x}$	$\Gamma_3 \oplus \Gamma_7$	Γ_5
$10/mmm$	$\sim 10\,22 \times \mathbb{Z}_2$	$\Gamma_{2u} \oplus \Gamma_{5u}$	Γ_{7u}

(*g*) C_{12} [$\omega = \exp(\pi i/6)$].

C_{12}	ε	α	α^2	α^3	α^4	α^5
n	1	1	1	1	1	1
Order	1	12	6	4	3	12
Γ_1	1	1	1	1	1	1
Γ_2	1	ω	ω^2	i	ω^4	ω^5
Γ_3	1	ω^2	ω^4	-1	$-\omega^2$	$-\omega^4$
Γ_4	1	i	-1	$-i$	1	i
Γ_5	1	ω^4	$-\omega^2$	1	ω^4	$-\omega^2$
Γ_6	1	ω^5	$-\omega^4$	i	$-\omega^2$	ω
Γ_7	1	-1	1	-1	1	-1
Γ_8	1	$-\omega$	ω^2	$-i$	ω^4	$-\omega^5$
Γ_9	1	$-\omega^2$	ω^4	1	$-\omega^2$	ω^4
Γ_{10}	1	$-i$	-1	i	1	$-i$
Γ_{11}	1	$-\omega^4$	$-\omega^2$	-1	ω^4	ω^2
Γ_{12}	1	$-\omega^5$	$-\omega^4$	$-i$	$-\omega^2$	$-\omega$

C_{12}	α^6	α^7	α^8	α^9	α^{10}	α^{11}
n	1	1	1	1	1	1
Order	2	12	3	4	6	12
Γ_1	1	1	1	1	1	1
Γ_2	-1	$-\omega$	$-\omega^2$	$-i$	$-\omega^4$	$-\omega^5$
Γ_3	1	ω^2	ω^4	-1	$-\omega^2$	$-\omega^4$
Γ_4	-1	$-i$	1	i	-1	$-i$
Γ_5	1	ω^4	$-\omega^2$	1	ω^4	$-\omega^2$
Γ_6	-1	$-\omega^5$	ω^4	$-i$	ω^2	$-\omega$
Γ_7	1	-1	1	-1	1	-1
Γ_8	-1	ω	$-\omega^2$	i	$-\omega^4$	ω^5
Γ_9	-1	ω^5	ω^4	i	ω^2	ω

	Generators	Vector representation	Perpendicular representation
$\underline{12}$ $\overline{12}$	$\alpha = C_{12z}$ $\alpha = S_{12z}$	$\Gamma_1 \oplus \Gamma_2 \oplus \Gamma_{12}$ $\Gamma_6 \oplus \Gamma_7 \oplus \Gamma_8$	$\Gamma_6 \oplus \Gamma_8$ $\Gamma_2 \oplus \Gamma_{12}$
$12/m$	$\sim 12 \times \mathbb{Z}_2$	$\Gamma_{1u} \oplus \Gamma_{2u} \oplus \Gamma_{12u}$	$\Gamma_{6u} \oplus \Gamma_{8u}$

(*h*) D_{12}

D_{12}	ε	α	α^2	α^3
n	1	2	2	2
Order	1	12	6	4
Γ_1	1	1	1	1
Γ_2	1	1	1	1
Γ_3	1	-1	1	-1
Γ_4	1	-1	1	-1
Γ_5	2	$\sqrt{3}$	1	0
Γ_6	2	1	-1	-2
Γ_7	2	0	-2	0
Γ_8	2	-1	-1	2
Γ_9	2	$-\sqrt{3}$	1	0

D_{12}	α^4	α^5	α^6	β	$\alpha\beta$
n	2	2	1	6	6
Order	3	12	2	2	2
Γ_1	1	1	1	1	1
Γ_2	1	1	1	-1	-1
Γ_3	1	-1	1	1	-1
Γ_4	1	-1	1	-1	1
Γ_5	-1	$-\sqrt{3}$	-2	0	0
Γ_6	-1	1	2	0	0
Γ_7	2	0	-2	0	0
Γ_8	-1	-1	2	0	0
Γ_9	-1	$\sqrt{3}$	-2	0	0

	Generators	Vector representation	Perpendicular representation
$12\,22$	$\alpha = C_{12z}$ $\beta = C_{2x}$	$\Gamma_2 \oplus \Gamma_5$	Γ_9
$12\,mm$	$\alpha = C_{12z}$ $\beta = m_x$	$\Gamma_1 \oplus \Gamma_5$	Γ_9
$\overline{12}\,2m$	$\alpha = S_{12z}$ $\beta = C_{2x}$	$\Gamma_4 \oplus \Gamma_9$	Γ_5
$12/mmm$	$\sim 12\,22 \times \mathbb{Z}_2$	$\Gamma_{2u} \oplus \Gamma_{5u}$	Γ_{9u}

(*i*) I [$\tau = (\sqrt{5}-1)/2$].

I	ε	α	α^2	β	$\alpha\beta$
n	1	12	12	20	15
Order	1	5	5	3	2
Γ_1	1	1	1	1	1
Γ_2	3	$1+\tau$	$-\tau$	0	-1
Γ_3	3	$-\tau$	$1+\tau$	0	-1
Γ_4	4	-1	-1	1	0
Γ_5	5	0	0	-1	1

	Generators	Vector representation	Perpendicular representation
532	$\alpha = C_5$ $\beta = C_{3d}$	Γ_2	Γ_3
$\bar{5}\bar{3}m$	$\sim 532 \times \mathbb{Z}_2$	Γ_{2u}	Γ_{3u}

Table 1.10.5.2. *Matrices of the irreducible representations of dimension $d \geq 2$ corresponding to the irreps of Table 1.10.5.1*

(a) D_5

Representation	$D(\alpha^p)$	$D(\beta)$
Γ_3	$\begin{pmatrix} \cos(2\pi p/5) & -\sin(2\pi p/5) \\ \sin(2\pi p/5) & \cos(2\pi p/5) \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
Γ_4	$\begin{pmatrix} \cos(4\pi p/5) & -\sin(4\pi p/5) \\ \sin(4\pi p/5) & \cos(4\pi p/5) \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

(b) D_8

Representation	$D(\alpha^p)$	$D(\beta)$
Γ_5	$\begin{pmatrix} \cos(\pi p/4) & -\sin(\pi p/4) \\ \sin(\pi p/4) & \cos(\pi p/4) \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
Γ_6	$\begin{pmatrix} \cos(\pi p/2) & -\sin(\pi p/2) \\ \sin(\pi p/2) & \cos(\pi p/2) \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
Γ_7	$\begin{pmatrix} \cos(3\pi p/4) & -\sin(3\pi p/4) \\ \sin(3\pi p/4) & \cos(3\pi p/4) \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

(c) D_{10}

Representation	$D(\alpha^p)$	$D(\beta)$
Γ_5	$\begin{pmatrix} \cos(\pi p/5) & -\sin(\pi p/5) \\ \sin(\pi p/5) & \cos(\pi p/5) \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
Γ_6	$\begin{pmatrix} \cos(2\pi p/5) & -\sin(2\pi p/5) \\ \sin(2\pi p/5) & \cos(2\pi p/5) \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
Γ_7	$\begin{pmatrix} \cos(3\pi p/5) & -\sin(3\pi p/5) \\ \sin(3\pi p/5) & \cos(3\pi p/5) \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
Γ_8	$\begin{pmatrix} \cos(4\pi p/5) & -\sin(4\pi p/5) \\ \sin(4\pi p/5) & \cos(4\pi p/5) \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

(d) D_{12}

Representation	$D(\alpha^p)$	$D(\beta)$
Γ_5	$\begin{pmatrix} \cos(\pi p/6) & -\sin(\pi p/6) \\ \sin(\pi p/6) & \cos(\pi p/6) \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
Γ_6	$\begin{pmatrix} \cos(\pi p/3) & -\sin(\pi p/3) \\ \sin(\pi p/3) & \cos(\pi p/3) \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
Γ_7	$\begin{pmatrix} \cos(\pi p/2) & -\sin(\pi p/2) \\ \sin(\pi p/2) & \cos(\pi p/2) \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
Γ_8	$\begin{pmatrix} \cos(2\pi p/3) & -\sin(2\pi p/3) \\ \sin(2\pi p/3) & \cos(2\pi p/3) \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
Γ_9	$\begin{pmatrix} \cos(5\pi p/6) & -\sin(5\pi p/6) \\ \sin(5\pi p/6) & \cos(5\pi p/6) \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

Table 1.10.5.1 gives the characters of the point groups C_n with $n = 5, 8, 10, 12$, D_n with $n = 5, 8, 10, 12$, and the icosahedral group I. The direct products with $\mathbb{Z}_2$ then follow easily. Although these direct products of a group K with $\mathbb{Z}_2$ do not belong to the isomorphism class of K, their irreducible representations are nevertheless given in the table for K because these irreducible representations have the same labels as those for K apart from an additional subindex u. The reresentations of the subgroup K of $K \times \mathbb{Z}_2$ are the same as for K itself, those for the cosets get an additional minus sign. In the tables, the characters for the groups $K \times \mathbb{Z}_2$ are separated from those for K by a horizontal rule. In addition to the characters are given the realizations of crystallographic point groups, and the irreducible components of the vector representations in direct space V_E and internal space V_I for these realizations. The vector representation in V_I is called the perpendicular representation.

In Table 1.10.5.2 the representation matrices for the irreducible representations in more than one dimension are given (one-dimensional representations are just the characters). For the cyclic groups there are only one-dimensional representations, for the dihedral groups there are one- and two-dimensional irreducible representations. There are four irreducible representations of I of dimension larger than one. The four- and five-dimensional ones are given as integer representations. They form

Table 1.10.5.2 (*cont.*)

(*e*) *I*. First column: numbering of the elements. $f = (1+\sqrt{5})/2$, $t = (\sqrt{5}-1)/2$. Horizontal rules separate conjugation classes.

No.	Order	Γ_2	Γ_4	Γ_5
1	1	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$
2	5	$\begin{pmatrix} 1/2 & t/2 & -f/2 \\ t/2 & f/2 & 1/2 \\ f/2 & -1/2 & t/2 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 1 & -1 \end{pmatrix}$
3	5	$\begin{pmatrix} 1/2 & -t/2 & f/2 \\ -t/2 & f/2 & 1/2 \\ f/2 & -1/2 & t/2 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 & -1 \\ 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 1 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 \\ 1 & -1 & 0 & 0 & 0 \end{pmatrix}$
4	5	$\begin{pmatrix} 1/2 & t/2 & f/2 \\ t/2 & f/2 & -1/2 \\ -f/2 & 1/2 & t/2 \end{pmatrix}$	$\begin{pmatrix} -1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & -1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 & 1 \\ 0 & -1 & 0 & 0 & 0 \end{pmatrix}$
5	5	$\begin{pmatrix} t/2 & -f/2 & 1/2 \\ f/2 & 1/2 & t/2 \\ -1/2 & t/2 & f/2 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 1 \\ 1 & -1 & 0 & 0 \\ 0 & -1 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & -1 & 0 \\ 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 & 0 \end{pmatrix}$
6	5	$\begin{pmatrix} f/2 & -1/2 & -t/2 \\ 1/2 & t/2 & f/2 \\ -t/2 & -f/2 & 1/2 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & -1 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & 1 \\ 1 & 0 & -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}$
7	5	$\begin{pmatrix} f/2 & 1/2 & t/2 \\ -1/2 & t/2 & f/2 \\ t/2 & -f/2 & 1/2 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 0 & 1 \\ 0 & -1 & 1 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 \end{pmatrix}$
8	5	$\begin{pmatrix} t/2 & f/2 & -1/2 \\ -f/2 & 1/2 & t/2 \\ 1/2 & t/2 & f/2 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 \\ -1 & 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 & 1 & -1 \\ 1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & 0 & -1 \end{pmatrix}$
9	5	$\begin{pmatrix} t/2 & f/2 & 1/2 \\ -f/2 & 1/2 & -t/2 \\ -1/2 & -t/2 & f/2 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & 1 & -1 & 0 \\ 1 & 0 & -1 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 & 1 & 0 \\ -1 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 \end{pmatrix}$
10	5	$\begin{pmatrix} f/2 & 1/2 & -t/2 \\ -1/2 & t/2 & -f/2 \\ -t/2 & f/2 & 1/2 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 0 & 1 \\ 1 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & -1 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix}$
11	5	$\begin{pmatrix} 1/2 & -t/2 & -f/2 \\ -t/2 & f/2 & -1/2 \\ f/2 & 1/2 & t/2 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & -1 & 0 \\ 0 & 0 & -1 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & -1 & 0 & 0 \\ 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 1 & -1 & 0 & 0 \end{pmatrix}$
12	5	$\begin{pmatrix} f/2 & -1/2 & t/1 \\ 1/2 & t/2 & -f/2 \\ t/2 & f/2 & 1/2 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & -1 \\ 1 & 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & -1 & 0 \end{pmatrix}$

Table 1.10.5.2 (*cont.*)

No.	Order	Γ_2	Γ_4	Γ_5
13	5	$\begin{pmatrix} t/2 & -f/2 & -1/2 \\ f/2 & 1/2 & -t/2 \\ 1/2 & -t/2 & f/2 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 & 1 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 \end{pmatrix}$
14	5	$\begin{pmatrix} -t/2 & f/2 & -1/2 \\ f/2 & 1/2 & t/2 \\ 1/2 & -t/2 & -f/2 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & -1 & 1 \\ 0 & 0 & -1 & 0 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & -1 & 0 \end{pmatrix}$
15	5	$\begin{pmatrix} -t/2 & f/2 & 1/2 \\ f/2 & 1/2 & -t/2 \\ -1/2 & t/2 & -f/2 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 \end{pmatrix}$
16	5	$\begin{pmatrix} -f/2 & 1/2 & -t/2 \\ -1/2 & -t/2 & f/2 \\ t/2 & f/2 & 1/2 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & -1 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 1 \\ 1 & -1 & 0 & 0 & 0 \end{pmatrix}$
17	5	$\begin{pmatrix} -t/2 & -f/2 & 1/2 \\ -f/2 & 1/2 & t/2 \\ -1/2 & -t/2 & -f/2 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 1 & -1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 1 & 0 & -1 \end{pmatrix}$
18	5	$\begin{pmatrix} -t/2 & -f/2 & -1/2 \\ -f/2 & 1/2 & -t/2 \\ 1/2 & t/2 & -f/2 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 & 0 \end{pmatrix}$
19	5	$\begin{pmatrix} -f/2 & -1/2 & t/2 \\ 1/2 & -t/2 & f/2 \\ -t/2 & f/2 & 1/2 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 \end{pmatrix}$
20	5	$\begin{pmatrix} -f/2 & 1/2 & t/2 \\ -1/2 & -t/2 & -f/2 \\ -t/2 & -f/2 & 1/2 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 1 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & -1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{pmatrix}$
21	5	$\begin{pmatrix} 1/2 & -t/2 & f/2 \\ t/2 & -f/2 & -1/2 \\ f/2 & 1/2 & -t/2 \end{pmatrix}$	$\begin{pmatrix} -1 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 & 1 & -1 \\ 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & -1 \\ 1 & 0 & 0 & 0 & -1 \end{pmatrix}$
22	5	$\begin{pmatrix} 1/2 & -t/2 & -f/2 \\ t/2 & -f/2 & 1/2 \\ -f/2 & -1/2 & -t/2 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & -1 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix}$
23	5	$\begin{pmatrix} 1/2 & t/2 & f/2 \\ -t/2 & -f/2 & 1/2 \\ f/2 & -1/2 & -t/2 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & -1 & 0 \\ 1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & 1 & -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & -1 & 0 & 1 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \end{pmatrix}$
24	5	$\begin{pmatrix} 1/2 & t/2 & -f/2 \\ -t/2 & -f/2 & -1/2 \\ -f/2 & 1/2 & -t/2 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \\ -1 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$

Table 1.10.5.2 (*cont.*)

No.	Order	Γ_2	Γ_4	Γ_5
25	5	$\begin{pmatrix} -f/2 & -1/2 & -t/2 \\ 1/2 & -t/2 & -f/2 \\ t/2 & -f/2 & 1/2 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & -1 \\ 0 & 0 & 1 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 1 \end{pmatrix}$
26	3	$\begin{pmatrix} -1/2 & t/2 & -f/2 \\ -t/2 & f/2 & 1/2 \\ f/2 & 1/2 & -t/2 \end{pmatrix}$	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 & 1 \\ 1 & -1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \end{pmatrix}$
27	3	$\begin{pmatrix} -1/2 & -t/2 & f/2 \\ t/2 & f/2 & 1/2 \\ -f/2 & 1/2 & -t/2 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & -1 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 & -1 \\ 1 & 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & 0 & -1 \end{pmatrix}$
28	3	$\begin{pmatrix} -1/2 & t/2 & f/1 \\ -t/2 & f/2 & -1/2 \\ -f/2 & -1/2 & -t/2 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 \\ 1 & 0 & -1 & 0 & 0 \end{pmatrix}$
29	3	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & -1 \\ 1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 & -1 \end{pmatrix}$
30	3	$\begin{pmatrix} -1/2 & -t/2 & -f/2 \\ t/2 & f/2 & -1/2 \\ f/2 & -1/2 & -t/2 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 0 & 0 & 1 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 \end{pmatrix}$
31	3	$\begin{pmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & -1 & 1 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 1 & -1 \\ 0 & 1 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 & -1 \end{pmatrix}$
32	3	$\begin{pmatrix} f/2 & 1/2 & -t/2 \\ 1/2 & -t/2 & f/2 \\ t/2 & -f/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 1 & 0 \\ -1 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 & 1 \\ -1 & 0 & 1 & 0 & 0 \end{pmatrix}$
33	3	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 & -1 & 0 \\ 1 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & -1 & 0 \end{pmatrix}$
34	3	$\begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & -1 \\ 1 & 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 1 & 0 & -1 & 0 & 0 \end{pmatrix}$
35	3	$\begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 & 1 \\ -1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 & -1 & 1 \\ 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 0 & 1 & 0 & -1 & 0 \end{pmatrix}$
36	3	$\begin{pmatrix} f/2 & -1/2 & t/2 \\ -1/2 & -t/2 & f/2 \\ -t/2 & -f/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 0 & 0 & 1 \\ 0 & -1 & 0 & 1 & 0 \\ 1 & -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \end{pmatrix}$

Table 1.10.5.2 (*cont.*)

No.	Order	Γ_2	Γ_4	Γ_5
37	3	$\begin{pmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 \\ 1 & 0 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \end{pmatrix}$
38	3	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & -1 \\ 0 & 1 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 1 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \end{pmatrix}$
39	3	$\begin{pmatrix} f/2 & 1/2 & t/2 \\ 1/2 & -t/2 & -f/2 \\ -t/2 & f/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 1 & -1 & 0 \\ 1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 1 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 \end{pmatrix}$
40	3	$\begin{pmatrix} -t/2 & -f/2 & 1/2 \\ f/2 & -1/2 & -t/2 \\ 1/2 & t/2 & f/2 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 & 1 \\ -1 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 \end{pmatrix}$
41	3	$\begin{pmatrix} -t/2 & -f/2 & -1/2 \\ f/2 & -1/2 & t/2 \\ -1/2 & -t/2 & f/2 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & -1 & 1 & 0 \\ 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \end{pmatrix}$
42	3	$\begin{pmatrix} -t/2 & f/2 & 1/2 \\ -f/2 & -1/2 & t/2 \\ 1/2 & -t/2 & f/2 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & -1 & 1 \\ 1 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 & 0 \end{pmatrix}$
43	3	$\begin{pmatrix} -t/2 & f/2 & -1/2 \\ -f/2 & -1/2 & -t/2 \\ -1/2 & t/2 & f/2 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & -1 \end{pmatrix}$
44	3	$\begin{pmatrix} f/2 & -1/2 & -t/2 \\ -1/2 & -t/2 & -f/2 \\ t/2 & f/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 & 1 \\ 0 & 1 & 0 & -1 & 0 \\ 1 & 0 & 0 & -1 & 0 \end{pmatrix}$
45	3	$\begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 \\ -1 & 1 & 0 & 0 & 0 \end{pmatrix}$
46	2	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 & -1 \\ 1 & 0 & 0 & -1 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix}$
47	2	$\begin{pmatrix} -f/2 & 1/2 & t/2 \\ 1/2 & t/2 & f/2 \\ t/2 & f/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1 \\ -1 & 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$
48	2	$\begin{pmatrix} -f/2 & -1/2 & -t/2 \\ -1/2 & t/2 & f/2 \\ -t/2 & f/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 \\ -1 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 \end{pmatrix}$

Table 1.10.5.2 (*cont.*)

No.	Order	Γ_2	Γ_4	Γ_5
49	2	$\begin{pmatrix} -f/2 & -1/2 & t/2 \\ -1/2 & t/2 & -f/2 \\ t/2 & -f/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$
50	2	$\begin{pmatrix} -f/2 & 1/2 & -t/2 \\ 1/2 & t/2 & -f/2 \\ -t/2 & -f/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -1 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 & -1 & 1 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & -1 & 0 \end{pmatrix}$
51	2	$\begin{pmatrix} t/2 & f/2 & -1/2 \\ f/2 & -1/2 & -t/2 \\ -1/2 & -t/2 & -f/2 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 \\ -1 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 \\ -1 & 1 & 0 & 0 & 0 \end{pmatrix}$
52	2	$\begin{pmatrix} t/2 & f/2 & 1/2 \\ f/2 & -1/2 & t/2 \\ 1/2 & t/2 & -f/2 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 0 & 1 & -1 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & -1 & 0 & 0 \\ 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 0 & 1 \end{pmatrix}$
53	2	$\begin{pmatrix} -1/2 & t/2 & f/2 \\ t/2 & -f/2 & 1/2 \\ f/2 & 1/2 & t/2 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & -1 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}$
54	2	$\begin{pmatrix} -1/2 & t/2 & -f/2 \\ t/2 & -f/2 & -1/2 \\ -f/2 & -1/2 & t/2 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & -1 & 1 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & -1 & 0 \\ 1 & 0 & -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 & 0 & -1 \\ 0 & 1 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix}$
55	2	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 0 & 1 \\ 0 & -1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 1 & -1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 1 \end{pmatrix}$
56	2	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 \\ -1 & 0 & 1 & 0 \\ -1 & 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 1 \\ 0 & -1 & 0 & 1 & 0 \\ 0 & -1 & 1 & 0 & 0 \end{pmatrix}$
57	2	$\begin{pmatrix} -1/2 & -t/2 & -f/2 \\ -t/2 & -f/2 & 1/2 \\ -f/2 & 1/2 & t/2 \end{pmatrix}$	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & -1 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & -1 & 1 & 0 \end{pmatrix}$
58	2	$\begin{pmatrix} t/2 & -f/2 & -1/2 \\ -f/2 & -1/2 & t/2 \\ -1/2 & t/2 & -f/2 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & -1 & 0 \\ 1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{pmatrix}$
59	2	$\begin{pmatrix} t/2 & -f/2 & 1/2 \\ -f/2 & -1/2 & -t/2 \\ 1/2 & -t/2 & -f/2 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 & -1 \\ 0 & 1 & 0 & -1 \\ 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 1 & 0 & -1 \\ 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix}$
60	2	$\begin{pmatrix} -1/2 & -t/2 & f/2 \\ -t/2 & -f/2 & -1/2 \\ f/2 & -1/2 & t/2 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix}$

Table 1.10.5.3. *The representation matrices for* Γ_3

The representation matrices for Γ_3 are the same as for Γ_2. Correspondences are given as pairs i, j: $\Gamma_3(R_i) = \Gamma_2(R_j)$.

i	j	i	j	i	j	i	j	i	j	i	j
1	1	11	21	21	5	31	42	41	29	51	48
2	14	12	16	22	6	32	45	42	39	52	54
3	23	13	17	23	8	33	36	43	33	53	46
4	15	14	4	24	10	34	27	44	30	54	50
5	25	15	2	25	11	35	26	45	38	55	52
6	24	16	13	26	34	36	28	46	49	56	57
7	19	17	12	27	35	37	31	47	53	57	59
8	20	18	7	28	43	38	40	48	51	58	56
9	18	19	9	29	44	39	37	49	47	59	58
10	22	20	3	30	41	40	32	50	55	60	60

crystallographic groups in 4D and 5D. The two three-dimensional representations have the same matrices. The elements, however, are connected by an outer automorphism. That means that the ith element R_i is represented by $\Gamma_2(R_i)$ in the representation Γ_2, and by $\Gamma_3(R_i) = \Gamma_2(\varphi R_i)$ in Γ_3. The element φR_i is another element R_j. The corresponding j for each i is given in Table 1.10.5.3.

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