

1.10. TENSORS IN QUASIPERIODIC STRUCTURES

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

and consequently

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

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 $(\alpha_1 x, \dots, \alpha_n x)$ 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

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

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

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

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

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

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

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

One may define a function in n -dimensional space by

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

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}^* ($i = 1, 2, \dots, n$). 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

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

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.

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

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

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transformation R in V_E and an additional orthogonal transformation in V_I :

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

(1.10.2.7)

Moreover, there is the central inversion $-E$. The six-dimensional representation of the symmetry group, which is the icosahedral group $\bar{5}3m$, 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

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

(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

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

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

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

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.