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

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

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

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

1.10.3. Action of the symmetry group

1.10.3.1. *Action of superspace groups*

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

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

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

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

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

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

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

where the coefficient $Q_{\mathbf{k}\nu}$ is a normal coordinate, 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

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

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

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

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

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

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

$$g_{ij}' = \sum_{kl} R_{ki}R_{lj}g_{kl} = \sum_{kl} R_{ki}R_{lj}a_k^2\delta_{kl} = a_i^2\delta_{ij}$$

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 a given group of matrices $\Gamma(K)$. These are the coordinates in the space of invariant tensors.