International Tables for Crystallography (2006). Vol. D, Section 1.10.4.2, p. 250.

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

$$g = S^T g S, \qquad (1.10.4.5)$$

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

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

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

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

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

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

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

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

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

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

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-

  references