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1.2. Representations of crystallographic groups

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1.2.1. Introduction

Symmetry arguments play an important role in science. Often one can use them in a heuristic way, but the correct formulation is in terms of group theory. This remark is in fact superfluous for crystallographers, who are used to point groups and space groups as they occur in the description of structures. However, besides these structural problems there are many others where group theory may play a role. A central role in this context is played by representation theory, which treats the action of a group on physical quantities, and usually this is done in terms of linear transformations, although nonlinear representations may also occur.

To start with an example, consider a spin system, an arrangement of spins on sites with a certain symmetry, for example space-group symmetry. The elements of the space group map the sites onto other sites, but at the same time the spins are rotated or transformed otherwise in a well defined fashion. The spins can be seen as elements of a vector space (spin space) and the transformation in this space is an image of the space-group element. In a similar way, all symmetric tensors of rank 2 form a vector space, because one can add them and multiply them by a real factor. A linear change of coordinates changes the vectors, and the transformations in the space of tensors are the image of the coordinate transformations. Probably the most important use of such representations is in quantum mechanics, where transformations in coordinate space are mapped onto linear transformations in the quantum mechanical space of state vectors.

To see the relation between groups of transformations and the use of their representations in physics, consider a tensor which transforms under a certain point group. Let us take a symmetric rank 2 tensor T_{ij} in three dimensions. We take as example the point group 222. From Section 1.1.3.2 one knows how such a tensor transforms: it transforms into a tensor T'_{ij} according to

$$T'_{ij} = \sum_{k=1}^{3} \sum_{m=1}^{3} R_{ik} R_{jm} T_{km} \qquad (1.2.1.1)$$

for all orthogonal transformations R in the group 222. This action of the point group 222 is obviously a linear one:

$$\left(c_1 T_{ij}^{(1)} + c_2 T_{ij}^{(2)}\right)' = c_1 T_{ij}^{(1)\prime} + c_2 T_{ij}^{(2)\prime}.$$

The transformations on the tensors really form an image of the group, because if one writes $D(R)T$ for T', one has for two elements $R^{(1)}$ and $R^{(2)}$ the relation

$$\left(D(R^{(1)}R^{(2)})\right)T = D(R^{(1)})\left(D(R^{(2)})T\right)$$

or

$$D(R^{(1)}R^{(2)}) = D(R^{(1)})D(R^{(2)}). \qquad (1.2.1.2)$$

This property is said to define a (linear) representation. Because of the representation property, it is sufficient to know how the tensor transforms under the generators of a group. In our example, one could be interested in symmetric tensors that are invariant under the group 222. Then it is sufficient to consider the rotations over 180° along the x and y axes. If the point group is a symmetry group of the system, a tensor describing the relation between two physical quantities should remain the same. For invariant tensors one has

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

and the solution of these equations is

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{pmatrix} = \begin{pmatrix} a_{11} & 0 & 0 \\ 0 & a_{22} & 0 \\ 0 & 0 & a_{33} \end{pmatrix}.$$

The matrices of rank 2 form a nine-dimensional vector space. The rotation over 180° around the x axis can also be written as

$$R\begin{pmatrix} a_{11} \\ a_{12} \\ a_{13} \\ a_{21} \\ a_{22} \\ a_{23} \\ a_{31} \\ a_{32} \\ a_{33} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a_{11} \\ a_{12} \\ a_{13} \\ a_{21} \\ a_{22} \\ a_{23} \\ a_{31} \\ a_{32} \\ a_{33} \end{pmatrix}.$$

This nine-dimensional matrix together with the one corresponding to a rotation along the y axis generate a representation of the group 222 in the nine-dimensional space of three-dimensional rank 2 tensors. The invariant tensors form the subspace $(a_{11}, 0, 0, 0, a_{22}, 0, 0, 0, a_{33})$. In this simple case, group theory is barely needed. However, in more complex situations, the calculations may become quite cumbersome without group theory. Moreover, group theory may give a wealth of other information, such as selection rules and orthogonality relations, that can be obtained only with much effort without group theory, or in particular representation theory. Tables of tensor properties, and irreducible representations of point and space groups, have been in use for a long time. For point groups see, for example, Butler (1981) and Altmann & Herzig (1994); for space groups, see Miller & Love (1967), Kovalev (1987) and Stokes & Hatch (1988).

In the following, we shall discuss the representation theory of crystallographic groups. We shall adopt a slightly abstract language, which has the advantage of conciseness and generality, but we shall consider examples of the most important notions. Another point that could give rise to some problems is the fact that we shall consider in part the theory for crystallographic groups in arbitrary dimension. Of course, physics occurs in three-dimensional space, but often it is useful to see what is general and what is special for one, two or three dimensions. In Section 1.2.2, the point groups are discussed, together with their representations. In Section 1.2.3, the same is done for space groups. Tensors for point and space groups are then treated in terms of representation theory in Section 1.2.4. Besides transformations in space, transformations involving time reversal are important as well. They are discussed in Section 1.2.5. Information on crystallographic groups and their representations is presented in tabular form in Section 1.2.6. This section can be consulted independently.

1.2.2. Point groups

1.2.2.1. *Finite point groups in one, two and three dimensions*

The crystallographic point groups are treated in Volume A of *International Tables for Crystallography* (2005). Here we just give a brief summary of some important notions. To maintain generality, we consider the case of n-dimensional point groups.

Point groups in n dimensions are subgroups of the orthogonal group $O(n)$ in n dimensions. By definition they leave a point, the origin, invariant. They are of importance in physics because physical laws are invariant under such transformations. In this case $n = 1$, 2 or 3. For crystallography, the crystallographic point groups are the most relevant ones. A *crystallographic point group* is a subgroup of $O(n)$ that leaves an n-dimensional lattice invariant. A *lattice* is a collection of points

$$\mathbf{r} = \mathbf{r}_o + \sum_{i=1}^{n} n_i \mathbf{e}_i, \quad n_i \in \mathbb{Z}, \tag{1.2.2.1}$$

where the n vectors $\mathbf{e}_i$ form a basis of n-dimensional space. In other words, the points of the lattice can be obtained by the action of translations

$$\mathbf{t} = \sum_{i=1}^{n} n_i \mathbf{e}_i \tag{1.2.2.2}$$

on the lattice origin $\mathbf{r}_o$. These translations form a *lattice translation group* in n-dimensional space, *i.e.* a discrete subgroup of the group of all translations $T(n)$ in n dimensions, generated by n linearly independent translations.

Because a crystallographic point group leaves a lattice of points invariant, (a) it is a finite group of linear transformations and (b) on a basis of the lattice it is represented by integer matrices. On the other hand, as will be shown in Section 1.2.2.2, there is for every finite group of matrices an invariant scalar product, *i.e.* a positive definite metric tensor left invariant by the group. If one uses this metric tensor for the definition of the scalar product, the matrices represent orthogonal transformations. Moreover, when the matrices are integer, the group of matrices can be considered to be a crystallographic point group. In this sense, every finite group of integer matrices is a crystallographic point group. Consider as an example the group of matrices

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

which leaves invariant the metric tensor

$$g = \begin{pmatrix} \mathbf{a}_1\cdot\mathbf{a}_1 & \mathbf{a}_1\cdot\mathbf{a}_2 \\ \mathbf{a}_2\cdot\mathbf{a}_1 & \mathbf{a}_2\cdot\mathbf{a}_2 \end{pmatrix} = \begin{pmatrix} a & -a/2 \\ -a/2 & a \end{pmatrix}.$$

The lattice points $n_1\mathbf{a}_1 + n_2\mathbf{a}_2$ go over into lattice points and the transformation leaves the scalar product of two such vectors the same if the scalar product of the two vectors $n_1\mathbf{a}_1 + n_2\mathbf{a}_2$ and $n'_1\mathbf{a}_1 + n'_2\mathbf{a}_2$ is defined as

$$n_1n'_1a - n_1n'_2a/2 - n_2n'_1a/2 + n_2n'_2a.$$

After a basis transformation,

$$\mathbf{e}_1 = \mathbf{a}_1/\sqrt{a}, \quad \mathbf{e}_2 = (\mathbf{a}_1 + 2\mathbf{a}_2)/\sqrt{3a},$$

the metric tensor is in standard form (see Section 1.1.2.2):

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}.$$

This means that with respect to the basis $\mathbf{e}_1$, $\mathbf{e}_2$, the three transformations become orthogonal matrices.

To be able to give a list of all crystallographic point groups in n dimensions it is necessary to state which point groups should be considered as different. Two point groups belong to the same *geometric crystal class* if they are conjugated subgroups of $O(n)$. This means that $K \subset O(n)$ and $K' \subset O(n)$ belong to the same class if there is an element $R \in O(n)$ such that $K' = RKR^{-1}$, which implies that there are two orthonormal bases in the vector space related by an orthogonal transformation R such that the matrices of K for one basis are the same as those for K' on the second basis.

In *one-dimensional space*, there are only two different point groups, the first consisting of the identity, the second of the numbers ±1. These groups are isomorphic to C_1 and C_2, respectively, where C_m is the cyclic group of integers modulo m (also denoted by $\mathbb{Z}_m$). Both are crystallographic because their 1×1 'matrices' are the integers ±1.

In *two-dimensional space*, the orthogonal group $O(2)$ is the union of the subgroup $SO(2)$, consisting of all orthogonal transformations with determinant $+1$, and the coset $O(2)\backslash SO(2)$, consisting of all orthogonal transformations with determinant -1. The group $SO(2)$ is Abelian, and therefore all its subgroups are Abelian. The finite ones are the rotation groups denoted by n ($n \in \mathbb{Z}^+$). Every element of $O(2)\backslash SO(2)$ is of order two, and corresponds to a mirror line. Therefore, all the other finite point groups are nmm (n even) or nm (n odd). The rotation groups are isomorphic with the cyclic groups C_n and the others with the dihedral groups D_n. Only the groups 1, 2, 3, 4, 6, m, $2mm$, $3m$, $4mm$ and $6mm$ leave a lattice invariant and are crystallographic.

The isomorphism class of a group can be given by its *generators* and *defining relations*. For example, the elements of the group $4mm$ can be written as products (with generally more than two factors) of the two matrices

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

which satisfy the relations $A^4 = B^2 = ABAB = E$, and every group whose elements are products of two generating elements with the same and not more independent relations is isomorphic. One calls the relations the defining relations. The set of generators and defining relations is not unique. In an extreme case, one can consider all elements of the group as generators, and the product rules $ab = c$ as the defining relations.

For the two-dimensional groups, the generators and defining relations are

C_n: one generator A, with $A^n = E$;

D_n: two generators A and B, with $A^n = B^2 = (AB)^2 = E$, where E is the unit element.

The determination of all finite point groups in *three-dimensional space* is more involved. A derivation can, for example, be found in Janssen (1973). The group $O(3)$ is again the union of $SO(3)$ and $O(3)\backslash SO(3)$, and in fact the direct product of $SO(3)$ and the group generated by the inversion $I = -E$. One may distinguish between three different classes of finite point groups:

(a) point groups that belong fully to the rotation group $SO(3)$;

(b) point groups that contain the inversion $-E$ and are, consequently, the direct product of a point group of the first class and the group generated by $-E$;