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$$\Gamma(A)^3 = \Gamma(B)^2 = (\Gamma(A)\Gamma(B))^2 = E$$

and, consequently, this representation has a trivial factor system. This shows that, although 32^d has three extra representations, there are no nontrivial projective representations.

The characters for the double point groups are given in Table 1.2.6.7.

1.2.3. Space groups

1.2.3.1. *Structure of space groups*

The Euclidean group $E(n)$ in n dimensions is the group of all distance-preserving inhomogeneous linear transformations. In Euclidean space, an element is denoted by

$$g = \{R|\mathbf{a}\}$$

where $R \in O(n)$ and $\mathbf{a}$ is an n-dimensional translation. On a point $\mathbf{r}$ in n-dimensional space, g acts according to

$$\{R|\mathbf{a}\}\mathbf{r} = R\mathbf{r} + \mathbf{a}. \qquad (1.2.3.1)$$

Therefore, $|g\mathbf{r}_1 - g\mathbf{r}_2| = |\mathbf{r}_1 - \mathbf{r}_2|$. The group multiplication law is given by

$$\{R|\mathbf{a}\}\{R'|\mathbf{a}'\} = \{RR'|\mathbf{a} + R\mathbf{a}'\}. \qquad (1.2.3.2)$$

The elements $\{E|\mathbf{a}\}$ form an Abelian subgroup, the group of n-dimensional translations $T(n)$.

An n-dimensional space group is a subgroup of $E(n)$ such that its intersection with $T(n)$ is generated by n linearly independent basis translations. This means that this *lattice translation subgroup* A is isomorphic to the group of n-tuples of integers: each translation in A can be written as

$$\{E|\mathbf{a}\} = \prod_{i=1}^{n} \{E|\mathbf{e}_i\}^{n_i} = \{E|\sum_{i=1}^{n} n_i \mathbf{e}_i\}. \qquad (1.2.3.3)$$

The lattice translation subgroup A is an invariant subgroup because

$$g\{E|\mathbf{a}\}g^{-1} = \{R|\mathbf{b}\}\{E|\mathbf{a}\}\{R|\mathbf{b}\}^{-1} = \{E|R\mathbf{a}\} \in A.$$

The factor group G/A, of the space group G and the lattice translation group A, is isomorphic to the group K formed by all elements R occurring in the elements $\{R|\mathbf{a}\} \in G$. This group is the *point group* of the space group G. It is a subgroup of $O(n)$.

The *unit cell* of the space group is a domain in n-dimensional space such that every point in space differs by a lattice translation from some point in the unit cell, and such that between any two points in the unit cell the difference is not a lattice translation. The unit cell is not unique. One choice is the n-dimensional parallelepiped spanned by the n basis vectors. The points in this unit cell have coordinates between 0 (inclusive) and 1. Another choice is not basis dependent: consider all points generated by the lattice translation group from an origin. This produces a lattice of points Λ. Consider now all points that are closer to the origin than to any other lattice point. This domain is a unit cell, if one takes care which part of the boundary belongs to it and which part not, and is called the *Wigner–Seitz cell*. In mathematics it is called the *Voronoi cell* or *Dirichlet domain* (or region).

Because the point group leaves the lattice of points invariant, it transforms the Wigner–Seitz cell into itself. This implies that points inside the unit cell may be related by a point-group element. Similarly, space-group elements may connect points inside the unit cell, up to lattice translations. A *fundamental region* or *asymmetric unit* is a part of the unit cell such that no points of the fundamental region are connected by a space-group element, and simultaneously that any point in space can be related to a point in the fundamental region by a space-group transformation.

Because $\{E|R\mathbf{a}\}$ belongs to the lattice translation group for every $R \in K$ and every lattice translation $\{E|\mathbf{a}\}$, the lattice Λ generated by the vectors $\mathbf{e}_i$ ($i = 1, 2, \ldots, n$) is invariant under the point group K. Therefore, the latter is a crystallographic point group. On a basis of the lattice Λ, the point group corresponds to a group $\Gamma(K)$ of integer matrices. One has the following situation. The space group G has an invariant subgroup A isomorphic to $\mathbb{Z}^n$, the factor group G/A is a crystallographic point group K which acts according to the integer representation $\Gamma(K)$ on A. In mathematical terms, G is an *extension* of K by A with homomorphism Γ from K to the group of automorphisms of A.

The vectors $\mathbf{a}$ occurring in the elements $\{E|\mathbf{a}\} \in G$ are called primitive translations. They have integer coefficients with respect to the basis $\mathbf{e}_1, \ldots, \mathbf{e}_n$. However, not all vectors $\mathbf{a}$ in the space-group elements are necessarily primitive. One can decompose the space group G according to

$$G = A + g_2A + g_3A + \ldots + g_NA. \qquad (1.2.3.4)$$

To every element $R \in K$ there is a coset g_iA with $g_i = \{R|\mathbf{a}(R)\}$ as representative. Such a representative is unique up to a lattice translation. Instead of $\mathbf{a}(R)$, one could as well have $\mathbf{a}(R) + \mathbf{n}$ as representative for any lattice translation $\mathbf{n}$. For a particular choice, the function $\mathbf{a}(R)$ from the point group to the group $T(n)$ is called the *system of nonprimitive translations* or *translation vector system*. It is a mapping from the point group K to $T(n)$, modulo A. Such a system of nonprimitive translations satisfies the relations

$$\mathbf{a}(R) + R\mathbf{a}(S) = \mathbf{a}(RS) \bmod A \quad \forall\, R, S \in K. \qquad (1.2.3.5)$$

This follows immediately from the product of two representatives g_i.

If the lattice translation subgroup A acts on a point $\mathbf{r}$, one obtains the set $\Lambda + \mathbf{r}$. One can describe the elements of G as well as combinations of an orthogonal transformation with $\mathbf{r}$ as centre and a translation. This can be seen from

$$\{R|\mathbf{a}\} = \{E|\mathbf{a} - \mathbf{r} + R\mathbf{r}\}\{R|\mathbf{r} - R\mathbf{r}\}, \qquad (1.2.3.6)$$

where now $\{R|\mathbf{r} - R\mathbf{r}\}$ leaves the point $\mathbf{r}$ invariant. The new system of nonprimitive translations is given by

$$\mathbf{a}'(R) = \mathbf{a}(R) + (R - E)\mathbf{r}. \qquad (1.2.3.7)$$

This is the effect of a *change of origin*. Therefore, for a space group, the systems of nonprimitive translations are only determined up to a primitive translation and up to a change of origin.

It is often convenient to describe a space group on another basis, the conventional lattice basis. This is the basis for a sublattice with the same, or higher, symmetry and with the same number of free parameters. Therefore, the sublattice is also invariant under K and with respect to the conventional basis, which is obtained from the original one *via* a basis transformation S, the point group has the form

$$\Gamma_{\rm conventional}(R) = S\Gamma_{\rm primitive}(R)S^{-1}, \qquad (1.2.3.8)$$

where S is the *centring matrix*. It is a matrix with determinant equal to the inverse of the number of lattice points of the primitive lattice inside the unit cell of the conventional lattice. As an example, consider the primitive and centred rectangular lattices in two dimensions. Both have symmetry $2mm$, and two parameters a and b. The transformation from a basis of the conventional lattice $[(2a, 0)$ and $(0, 2b)]$ to a basis of the primitive lattice $[(a, -b)$ and $(a, b)]$ is given by S, and the relations between the generators of the point groups are

$$\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix} = S\begin{pmatrix}0 & -1\\ -1 & 0\end{pmatrix}S^{-1}, \quad S = \begin{pmatrix}\frac{1}{2} & \frac{1}{2}\\ -\frac{1}{2} & \frac{1}{2}\end{pmatrix}$$
$$\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = S\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}S^{-1}.$$

1.2.3.2. *Irreducible representations of lattice translation groups*

The lattice translation group A is isomorphic to the group $\mathbb{Z}^n$ of n-tuples of integers. This is an infinite group and, therefore, the usual techniques for finite groups cannot be applied. A way past this is the following. If $\mathbf{a}_i$ are the basis vectors of the lattice Λ, the lattice translation group generated by the translations $\{E|N\mathbf{a}_i\}$ forms an Abelian subgroup A^N of A. The factor group A/A^N is a finite group isomorphic to the direct product of n cyclic groups of order N. Each representation of this group is a representation of A with the property that the elements of A^N are represented by the unit operator. This procedure is in fact that of periodic boundary conditions in solid-state physics. In the following, we shall consider only the representations of A that satisfy this condition.

The irreducible representations of the direct product of n cyclic groups of order N are all one-dimensional. According to Section 1.2.2.6 they can be characterized by n integers and read

$$\Gamma^{\{p_j\}}\left(\{E|\sum_{i=1}^{n} n_i\mathbf{e}_i\}\right) = \exp[2\pi i(n_1p_1 + n_2p_2 + \ldots + n_np_n)/N], \tag{1.2.3.9}$$

because a representation of the cyclic group C_N is determined by its value on the basis translations:

$$\Gamma^p(\{E|\mathbf{e}\}) = \exp(2\pi ip/N), \quad 0 \le p < N.$$

There are exactly N^n nonequivalent irreducible representations.

If $\mathbf{a}_i$ are basis vectors of the lattice Λ, its dual basis consists of vectors $\mathbf{b}_j$ defined by

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}. \tag{1.2.3.10}$$

These vectors $\mathbf{b}_j$ span the *reciprocal lattice* Λ^*. The scalar product of an arbitrary lattice vector $\mathbf{a}$ and a reciprocal-lattice vectors $\mathbf{K}$ is then

$$\mathbf{K}\cdot\mathbf{a} = \left(\sum_{i=1}^{n} m_i\mathbf{b}_i\right)\cdot\left(\sum_{j=1}^{n} n_j\mathbf{a}_j\right) = 2\pi\sum_{i=1}^{n} n_im_i. \tag{1.2.3.11}$$

The expression (1.2.3.9) then can be written more concisely if one introduces an n-dimensional vector $\mathbf{k}$:

$$\mathbf{k} = (1/N)\sum_{i=1}^{n} p_i\mathbf{b}_i. \tag{1.2.3.12}$$

Then (1.2.3.9) simplifies to

$$\Gamma^{\{\mathbf{k}\}}(\{E|\mathbf{a}\}) = \exp(i\mathbf{k}\cdot\mathbf{a}). \tag{1.2.3.13}$$

Because $0 \le p_i/N < 1$, the vector $\mathbf{k}$ belongs to the unit cell of the reciprocal lattice. If one chooses that unit cell as the Voronoi cell for the reciprocal lattice, which in direct space would be the Wigner–Seitz cell, it is called the *Brillouin zone*. Therefore, representations of the lattice translation subgroup are characterized by a vector in the Brillouin zone. In fact, the vectors $\mathbf{k}$ form a mesh inside the Brillouin zone, but this mesh becomes finer if N increases. In the limit of N going to ∞, the wavevectors $\mathbf{k}$ fill the Brillouin zone.

Just like the direct lattice, the reciprocal lattice is invariant under the point group K. The Brillouin zone, or at least its interior, is invariant under K as well. A *fundamental domain* in the Brillouin zone is a part of the zone such that no two points of the fundamental region are related by a point-group transformation from K and that any point in the Brillouin zone can be obtained from a point in the fundamental region by a point-group transformation.

1.2.3.3. *Irreducible representations of space groups*

For representations of space groups, we use the same argumentation as for the lattice translation subgroup. Notice that the group A^N generated by the vectors $\{E|N\mathbf{e}_i\}$ is an invariant Abelian subgroup of the space group G as well.

$$\{R|\mathbf{a}\}\{E|N\mathbf{e}_i\}\{R^{-1}|-R^{-1}\mathbf{a}\} = \{E|NR\mathbf{e}_i\} \in A^N.$$

The factor group G/A^N is a finite group of order N^n times the order of the point group K. Representations of this factor group are representations of G with the property that all elements of A^N are mapped on the unit operator. We shall consider here only such space-group representations.

Suppose that $\Gamma(G)$ is an irreducible representation of the space group G. Its restriction $\Gamma(A)$ to the lattice translation subgroup is then reducible, unless it is one-dimensional. Each irreducible representation of A is characterized by a vector $\mathbf{k}$ in the Brillouin zone. Therefore,

$$\Gamma(\{E|\mathbf{a}\}) = \begin{pmatrix} \exp(i\mathbf{k}_1\cdot\mathbf{a}) & 0 & 0 & \ldots & 0 & 0\\ 0 & \exp(i\mathbf{k}_2\cdot\mathbf{a}) & 0 & \ldots & 0 & 0\\ 0 & 0 & \exp(i\mathbf{k}_3\cdot\mathbf{a}) & \ldots & 0 & 0\\ 0 & 0 & 0 & \ldots & \ldots & 0\\ 0 & 0 & 0 & \ldots & 0 & \exp(i\mathbf{k}_n\cdot\mathbf{a}) \end{pmatrix}. \tag{1.2.3.14}$$

Some of the vectors $\mathbf{k}_i$ may be identical. Therefore, the matrix representation can be written as

$$\Gamma(\{E|\mathbf{a}\}) = \begin{pmatrix} \exp(i\mathbf{k}_1\cdot\mathbf{a})E & 0 & 0 & \ldots & 0 & 0\\ 0 & \exp(i\mathbf{k}_2\cdot\mathbf{a})E & 0 & \ldots & 0 & 0\\ 0 & 0 & \exp(i\mathbf{k}_3\cdot\mathbf{a})E & \ldots & 0 & 0\\ 0 & 0 & 0 & \ldots & 0 & 0\\ 0 & 0 & 0 & \ldots & 0 & \exp(i\mathbf{k}_s\cdot\mathbf{a})E \end{pmatrix}. \tag{1.2.3.15}$$

It can be shown that the dimensions of the unit matrices E are all the same (and equal to d). Then

$$n = s\cdot d.$$

With respect to the basis on which the translation is of this form, every basis vector in the pth block is multiplied by a factor $\exp(i\mathbf{k}_p\cdot\mathbf{a})$.

Suppose that $\{R|\mathbf{u}\}$ is an element of the space group G. Consider a basis vector v of the representation space that gets a factor $\exp(i\mathbf{k}\cdot\mathbf{a})$ under the translation $\{E|\mathbf{a}\}$. Then one has

$$\begin{aligned} D(\{E|\mathbf{a}\})v &= \exp(i\mathbf{k}\cdot\mathbf{a})v\\ D(\{E|\mathbf{a}\})D(\{R|\mathbf{u}\})v &= D(\{R|\mathbf{u}\})D(\{E|R^{-1}\mathbf{a}\})v\\ &= \exp(iR\mathbf{k}\cdot\mathbf{a})D(\{R|\mathbf{u}\})v, \end{aligned}$$

and because $D(\{R|\mathbf{u}\})v$ also belongs to the representation space there are vectors that transform with the vector $R\mathbf{k}$ as well as vectors that transform with $\mathbf{k}$. This means that for every vector $\mathbf{k}$ occurring in a block in (1.2.3.5), there is also a block for each vector $R\mathbf{k}$ as R runs over the point group K. The vectors $\{R\mathbf{k}|R \in K\}$ form *the star of* $\mathbf{k}$. Vectors $R\mathbf{k}$ that differ by a reciprocal-lattice vector ($\mathbf{k}' = \mathbf{k} + \mathbf{K}$ with $K \in \Lambda^*$) correspond to the same representation and are therefore considered to be the same. Generally, a vector $\mathbf{k}$ may be left invariant by a subgroup of the point group K. This point group $K_{\mathbf{k}}$ is the *point group of* $\mathbf{k}$.

$$K_{\mathbf{k}} \equiv \{R|R\mathbf{k} \equiv \mathbf{k} \bmod \Lambda^*\}. \tag{1.2.3.16}$$

Then there are s point-group elements R_i such that

$$K = K_{\mathbf{k}} \cup R_2K_{\mathbf{k}} \cup \ldots \cup R_sK_{\mathbf{k}} \tag{1.2.3.17}$$

and each element R_i corresponds to a vector in the star:

$$\mathbf{k}_i = R_i\mathbf{k}_1; \quad \mathbf{k}_1 = \mathbf{k}, \quad i = 1, 2, \ldots, s.$$

Therefore, the blocks in (1.2.3.15) for an irreducible representation of the space group G correspond to the s branches of the star of $\mathbf{k}$. They are all of the same dimension d. If the vectors $\mathbf{k}_i$ in (1.2.3.15) belonged to two or more different stars, the representation would be reducible.

To the point group of $\mathbf{k}$ corresponds a subgroup of the space group G that has $K_{\mathbf{k}}$ as point group. It is called *the group of* $\mathbf{k}$ and is defined by

$$G_{\mathbf{k}} \equiv \{g = \{R|\mathbf{a}\} \in G|R \in K_{\mathbf{k}}\}. \tag{1.2.3.18}$$

Analogously to (1.2.3.17), one can write

$$G = G_{\mathbf{k}} \cup g_2G_{\mathbf{k}} \cup \ldots \cup g_sG_{\mathbf{k}} \tag{1.2.3.19}$$

for elements $g_i = \{R_i|\mathbf{a}_i\}$ of the space group G.

As one sees from (1.2.3.15), there is a subspace of vectors v that get a factor $\exp(i\mathbf{k}\cdot\mathbf{a})$ for any lattice translation $\mathbf{a}$. If one considers the action of $D(g)$ with $g \in G_{\mathbf{k}}$, it follows immediately that a vector from this space is transformed into a vector of the same space: the subspace corresponding to a vector $\mathbf{k}$ is invariant under $G_{\mathbf{k}}$. Therefore this space $V_{\mathbf{k}}$ carries a representation of $G_{\mathbf{k}}$. It can be seen as follows that one may construct the irreducible representation of the whole group G as soon as one knows the representation $D_{\mathbf{k}}$ of $G_{\mathbf{k}}$ in $V_{\mathbf{k}}$. To that end, consider a basis $\mathbf{e}_1, \ldots, \mathbf{e}_d$ in $V_{\mathbf{k}}$. The vectors

$$\boldsymbol{\psi}_{i\mu} = D(g_i)\mathbf{e}_\mu \quad (i = 1, 2, \ldots, s;\ \mu = 1, 2, \ldots, d), \tag{1.2.3.20}$$

form a basis of the whole representation space. Under a lattice-translation vector $\mathbf{a}$, the vector $\boldsymbol{\psi}_{i\mu}$ gets a factor $\exp(i\mathbf{k}_i\cdot\mathbf{a})$. On this basis, one can determine the matrix representation $\Gamma(G)$. Take an element $\{R|\mathbf{u}\} \in G$. It belongs to a certain coset $g_mG_{\mathbf{k}}$ in the decomposition of G. In addition, the element $\{R|\mathbf{u}\}g_i$ belongs to a well defined $g_jG_{\mathbf{k}}$. This means that there is an element $\{S|\mathbf{v}\}$ in the group $G_{\mathbf{k}}$ such that

$$\{R|\mathbf{u}\}g_i = g_j\{S|\mathbf{v}\} \quad (i = 1, 2, \ldots, s;\ \{S|\mathbf{v}\} \in G_{\mathbf{k}}).$$

Then one can write

$$\begin{aligned} D(\{R|\mathbf{u}\})\psi_{i\mu} &= D(\{R|\mathbf{u}\})D(g_i)\mathbf{e}_\mu \\ &= D(g_j)D(\{S|\mathbf{v}\})\mathbf{e}_\mu \\ &= D(g_j)\sum_{\nu=1}^{d}\Gamma_{\mathbf{k}}(\{S|\mathbf{v}\})_{\nu\mu}\mathbf{e}_\mu \\ &= \sum_{\nu=1}^{d}\Gamma_{\mathbf{k}}(\{S|\mathbf{v}\})_{\nu\mu}\psi_{j\nu} \\ &= \sum_{j=1}^{s}\sum_{\nu=1}^{d}\Gamma(\{R|\mathbf{u}\})_{j\nu,i\mu}\psi_{j\nu}. \end{aligned}$$

This means that the representation matrix $\Gamma(\{R|\mathbf{u}\})$ can be decomposed into $s \times s$ blocks of dimension d. In each row of blocks there is exactly one that is not a block of zeros, and the same is true for each column of blocks. Moreover, the only nonzero block in the ith column and in the jth row is

$$D_{\mathbf{k}}(\{S|\mathbf{v}\}) = D_{\mathbf{k}}(g_j^{-1}\{R|\mathbf{u}\}g_i), \tag{1.2.3.21}$$

where i and j are uniquely related by

$$\{R|\mathbf{u}\}g_i \in g_jG_{\mathbf{k}}. \tag{1.2.3.22}$$

It can be shown that $\Gamma(G)$ is irreducible if and only if $D_{\mathbf{k}}(G_{\mathbf{k}})$ is irreducible. From the construction, it is obvious that one may obtain all irreducible representations of G in this way. Moreover, one obtains all representations of G if one takes for the construction all stars and for each star all irreducible representations of $G_{\mathbf{k}}$.

So the final step is to determine all nonequivalent irreducible representations of $G_{\mathbf{k}}$. Notice that the lattice translation subgroup is a subgroup of $G_{\mathbf{k}}$. Therefore,

$$D_{\mathbf{k}}(\{E|\mathbf{a}\}) = \exp(i\mathbf{k}\cdot\mathbf{a})E.$$

If one makes a choice for the system of nonprimitive translations $\mathbf{u}(R)$, every element $g = \{S|\mathbf{v}\} \in G_{\mathbf{k}}$ can be written uniquely as

$$g = \{E|\mathbf{a}\}\{S|\mathbf{u}(S)\},$$

for a lattice translation $\mathbf{a}$. Therefore, one has

$$D_{\mathbf{k}}(\{S|\mathbf{v}\}) = \exp(i\mathbf{k}\cdot\mathbf{a})D_{\mathbf{k}}(\{S|\mathbf{u}(S)\}) \equiv \exp\{i\mathbf{k}\cdot[\mathbf{a} + \mathbf{u}(S)]\}\Gamma(S) \tag{1.2.3.23}$$

if one defines

$$\Gamma(S) = \exp[-i\mathbf{k}\cdot\mathbf{u}(S)]D_{\mathbf{k}}(\{S|\mathbf{u}(S)\}). \tag{1.2.3.24}$$

It is important to notice that this definition of Γ does not depend on the choice of the system of nonprimitive translations. If one takes $\mathbf{u}'(S) = \mathbf{u}(S) + \mathbf{b}$ ($\mathbf{b} \in A$), the result for $\Gamma(S)$ is the same. The product of two matrices $\Gamma(S)$ and $\Gamma(S')$ then becomes

$$\begin{aligned} \Gamma(S)\Gamma(S') &= \exp\bigl\{-i\mathbf{k}\cdot[\mathbf{u}(S) + \mathbf{u}(S')]\bigr\}D_{\mathbf{k}}(\{SS'|\mathbf{u}(S) + S\mathbf{u}(S')\}) \\ &= \exp\bigl\{-i\mathbf{k}\cdot[\mathbf{u}(S') - S\mathbf{u}(S')]\bigr\}\Gamma(SS'). \end{aligned} \tag{1.2.3.25}$$

One sees that the matrices $\Gamma(R)$ form a projective representation of the point group of $\mathbf{k}$. The factor system is given by

$$\begin{aligned} \omega(S, S') &= \exp\{-i\mathbf{k}\cdot[\mathbf{u}(S') - S\mathbf{u}(S')]\} \\ &= \exp[-i(\mathbf{k} - S^{-1})\cdot\mathbf{u}(S')]. \end{aligned} \tag{1.2.3.26}$$

Such a factor system may, however, be equivalent to a trivial one.

If the space group $G_{\mathbf{k}}$ is symmorphic, one may choose the system of nonprimitive translations to be zero. Consequently, in this case the factor system $\omega(S, S')$ is unity and the matrices $\Gamma(S)$ form an ordinary representation of the space group $G_{\mathbf{k}}$. This is also the case if $\mathbf{k}$ is not on the Brillouin-zone boundary. If $\mathbf{k}$ is inside the Brillouin zone and $S \in K_{\mathbf{k}}$, one has $S\mathbf{k} = \mathbf{k} + \mathbf{K}$ only for $\mathbf{K} = 0$. So inside the Brillouin zone one has $S\mathbf{k} = \mathbf{k}$ for all $S \in K_{\mathbf{k}}$. This implies that

$$\exp\{-i\mathbf{k}\cdot[\mathbf{u}(S') - S\mathbf{u}(S')]\} = \exp[-i(\mathbf{k} - S^{-1}\mathbf{k})\cdot\mathbf{u}(S')] = 1.$$

A nontrivial factor system $\omega(S, S')$ can therefore only occur for a nonsymmorphic group $G_{\mathbf{k}}$ and for a $\mathbf{k}$ on the Brillouin-zone boundary. But even then, it is possible that one may redefine the matrices $\Gamma(S)$ with an appropriate phase factor such that they form an ordinary representation. This is, for example, always the case if $K_{\mathbf{k}}$ is cyclic, because cyclic groups do not have genuine projective representations. These are always associated with an ordinary representation.

If the factor system $\omega(S, S')$ is not associated with a trivial one, one has to find the irreducible projective representations with the given factor system. As seen in the previous section, one may do this by using the defining relation for the point group $K_{\mathbf{k}}$. If these are words $W_i(A_1, \ldots, A_r)$ in the generators $A_1, \ldots, A_r$, the corresponding expressions in the representation

$$W_i(D_{\mathbf{k}}(A_1), \ldots, D_{\mathbf{k}}(A_r)) = \lambda_iE$$

are multiples of the unit operator. The values of λ_i fix the class of the factor system completely. By multiplying the operators $D_{\mathbf{k}}(A_j)$ by proper phase factors, the values of λ_i can be trans-

Table 1.2.3.1. *Choices of* **k** *in the fundamental domain of Pmmm and the elements of* $K_{\mathbf{k}}$

k	Wyckoff position	$K_{\mathbf{k}}$	Elements							
000	*a*	*mmm*	E	m_x	m_y	m_z	$\bar{1}$	2_x	2_y	2_z
$\frac{1}{2}00$	*b*	*mmm*	E	m_x	m_y	m_z	$\bar{1}$	2_x	2_y	2_z
$0\frac{1}{2}0$	*e*	*mmm*	E	m_x	m_y	m_z	$\bar{1}$	2_x	2_y	2_z
$00\frac{1}{2}$	*c*	*mmm*	E	m_x	m_y	m_z	$\bar{1}$	2_x	2_y	2_z
$0\frac{1}{2}\frac{1}{2}$	*g*	*mmm*	E	m_x	m_y	m_z	$\bar{1}$	2_x	2_y	2_z
$\frac{1}{2}0\frac{1}{2}$	*d*	*mmm*	E	m_x	m_y	m_z	$\bar{1}$	2_x	2_y	2_z
$\frac{1}{2}\frac{1}{2}0$	*f*	*mmm*	E	m_x	m_y	m_z	$\bar{1}$	2_x	2_y	2_z
$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	*h*	*mmm*	E	m_x	m_y	m_z	$\bar{1}$	2_x	2_y	2_z
$\xi00$	*i*	2*mm*	E	m_y	m_z	2_x				
$\xi\frac{1}{2}0$	*k*	2*mm*	E	m_y	m_z	2_x				
$\xi0\frac{1}{2}$	*j*	2*mm*	E	m_y	m_z	2_x				
$\xi\frac{1}{2}\frac{1}{2}$	*l*	2*mm*	E	m_y	m_z	2_x				
$0\eta0$	*m*	*m*2*m*	E	m_x	m_z	2_y				
$\frac{1}{2}\eta0$	*o*	*m*2*m*	E	m_x	m_z	2_y				
$0\eta\frac{1}{2}$	*n*	*m*2*m*	E	m_x	m_z	2_y				
$\frac{1}{2}\eta\frac{1}{2}$	*p*	*m*2*m*	E	m_x	m_z	2_y				
00ζ	*q*	*mm*2	E	m_x	m_y	2_z				
$\frac{1}{2}0\zeta$	*s*	*mm*2	E	m_x	m_y	2_z				
$0\frac{1}{2}\zeta$	*r*	*mm*2	E	m_x	m_y	2_z				
$\frac{1}{2}\frac{1}{2}\zeta$	*t*	*mm*2	E	m_x	m_y	2_z				
$0\eta\zeta$	*u*	*m*11	E	m_x						
$\frac{1}{2}\eta\zeta$	*v*	*m*11	E	m_x						
$\xi0\zeta$	*w*	1*m*1	E	m_y						
$\xi\frac{1}{2}\zeta$	*x*	1*m*1	E	m_y						
$\xi\eta0$	*y*	11*m*	E	m_z						
$\xi\eta\frac{1}{2}$	*z*	11*m*	E	m_z						
$\xi\eta\zeta$	α	1	E							

Table 1.2.3.2. *Strata of irreducible representations of Pmm*2 *and Pmmm*

k	Wyckoff position in *Pmm*2	Wyckoff positions in *Pmmm*	$K_{\mathbf{k}}$
00ζ	*a*	*a*, *c*, *q*	*mm*2
$0\frac{1}{2}\zeta$	*b*	*e*, *g*, *r*	*mm*2
$\frac{1}{2}0\zeta$	*c*	*b*, *d*, *s*	*mm*2
$\frac{1}{2}\frac{1}{2}\zeta$	*d*	*f*, *h*, *t*	*mm*2
$\xi0\zeta$	*e*	*i*, *j*, *w*	1*m*1
$\xi\frac{1}{2}\zeta$	*f*	*k*, *l*, *x*	1*m*1
$0\eta\zeta$	*g*	*m*, *n*, *u*	*m*11
$\frac{1}{2}\eta\zeta$	*h*	*o*, *p*, *v*	*m*11
$\xi\eta\zeta$	*i*	*y*, *z*, α	1

formed into those tabulated. Then the tables give all irreducible representations for this factor system.

In summary, the procedure for finding all irreducible representations of a space group G is as follows.

(1) Consider all stars of **k** with respect to G. This means that one takes all vectors **k** in a *fundamental region* of the Brillouin zone.

(2) For each star, one determines the group $K_{\mathbf{k}}$.

(3) For each $K_{\mathbf{k}}$, one determines the factor system $\omega(S, S')$.

(4) For this factor system, one looks for all nonequivalent irreducible (projective) representations.

(5) From the representations $D_{\mathbf{k}}(K_{\mathbf{k}})$, one determines the representations $\Gamma_{\mathbf{k}}(G_{\mathbf{k}})$ and $\Gamma(G)$ according to the procedure given above.

1.2.3.4. *Characterization of space-group representations*

The irreducible representations of space groups are characterized by a star of vectors in the Brillouin zone, and by the irreducible, possibly projective, representations of the point group of one point from that star.

The stars are sets of vectors in the Brillouin zone related mutually by transformations from the point group K of the space group G modulo reciprocal-lattice vectors. To obtain all stars, it is sufficient to take all vectors in the fundamental domain of the Brillouin zone, *i.e.* a part of the Brillouin zone such that no vectors in the domain are related by point-group elements (modulo Λ^*) and such that every point in the Brillouin zone is related to a vector in the fundamental domain by a point-group operation.

From each star one takes one point **k** and determines the nonequivalent irreducible representations of the point group $K_{\mathbf{k}}$, the ordinary representations if the group $G_{\mathbf{k}}$ is symmorphic or **k** is inside the Brillouin zone, or the projective representations with factor system ω [equation (1.2.3.26)] otherwise. These representations are labelled μ. There are several conventions for the choice of this label, but an irreducible representation of G is always characterized by a pair $(\mathbf{k}, \mu)$, where **k** fixes the star and μ the irreducible point-group representation.

The projective representations of the group of **k**, *i.e.* of $K_{\mathbf{k}}$, can be obtained from the ordinary representations of a larger group. If the factor system $\omega(R, R')$ is of order m [$\omega^m(R, R') = 1$ for all R, R'], the order of this larger group $\hat{K}_{\mathbf{k}\omega}$ is m times the order of $K_{\mathbf{k}}$. Then the irreducible representations of the space group are labelled by the vector **k** in the Brillouin zone and an irreducible ordinary representation of $\hat{K}_{\mathbf{k}\omega}$, where ω follows from (1.2.3.26).

Two stars such that one branch of the first one has the same $K_{\mathbf{k}}$ as one branch of the other determine representations that are quite similar. The only difference is the numerical value of the factors $\exp(i\mathbf{k}\cdot\mathbf{a})$, the form of the representation matrices being the same. Such irreducible representations of the space group are said to belong to the same *stratum*. Strata are denoted by a symbol for one vector **k** in the Brillouin zone. For example, the origin, conventionally denoted by Γ, belongs to one stratum that corresponds to the ordinary representations of the point group K. For a simple cubic space group, the point $[\frac{1}{2}, 0, 0]$ is denoted by X. Its $K_{\mathbf{k}}$ is the tetragonal group $4/mmm$. All points $[\xi, 0, 0]$ with $\xi \neq 0$ and $-\frac{1}{2} < \xi < \frac{1}{2}$ form one stratum with point group $4mm$. This stratum is denoted by Δ *etc*. The strata can be compared with the Wyckoff positions in direct space. There a Wyckoff position is a manifold in the unit cell for which all points have the same site symmetry, modulo the lattice translations. Here it is a manifold of k vectors with the same symmetry group modulo the reciprocal lattice. The action of $G_{\mathbf{k}}$ does not involve the nonprimitive translations. Therefore, the strata correspond to Wyckoff positions of the corresponding symmorphic space group. The stratum symbols for the various three-dimensional Bravais classes are given in Table 1.2.6.11.

As an example, we consider here the orthorhombic space group *Pnma*. The orthorhombic Brillouin zone has a fundamental domain with volume that is one-eighth of that of the Brillouin zone. The various choices of **k** in this fundamental domain, together with the corresponding point groups $K_{\mathbf{k}}$, are given in Table 1.2.3.1. The vectors **k** correspond to Wyckoff positions of the group *Pmmm*.

In the tables, the vectors **k** and their corresponding Wyckoff positions are given for the holohedral space groups. In general, the number of different strata is smaller for the other groups. One can still use the same symbols for these groups, or take the symbols for the Wyckoff positions for the groups that are not holohedral. Consider as an example the group *Pmm*2. Its holohedral space group is *Pmmm*. The strata of irreducible representations can be labelled by the symbols for Wyckoff positions of *Pmm*2 as well as those of *Pmmm*. This is shown in Table 1.2.3.2.

The defining relations for the point group *mmm* are

$$A^2 = B^2 = (AB)^2 = C^2 = E, \quad AC = CA, \quad BC = CB.$$

Table 1.2.3.3. *Characteristic values of λ_i for the projective irreps of $K_{\mathbf{k}}$ for the point group mmm*

	A^2	B^2	$(AB)^2$	C^2	$AC = CA$	$BC = CB$	Representations	
$\mathbf{k}$	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	Number	Dimension
000	1	1	1	1	1	1	8	1
$\frac{1}{2}00$	−1	1	−1	1	−1	1	2	2
$0\frac{1}{2}0$	1	−1	1	1	1	1	2	2
$00\frac{1}{2}$	1	1	1	−1	−1	1	2	2
$0\frac{1}{2}\frac{1}{2}$	1	−1	1	−1	−1	1	2	2
$\frac{1}{2}0\frac{1}{2}$	−1	1	−1	−1	1	1	8	1
$\frac{1}{2}\frac{1}{2}0$	−1	−1	−1	1	−1	1	2	2
$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	−1	−1	−1	−1	1	1	2	2
$\xi 00$	1	1	1				4	1
$\xi\frac{1}{2}0$	−1	1	−1				4	1
$\xi 0\frac{1}{2}$	1	−1	−1				4	1
$\xi\frac{1}{2}\frac{1}{2}$	−1	−1	1				4	1
$0\eta 0$	1	1	1				4	1
$\frac{1}{2}\eta 0$	−1	1	1				1	2
$0\eta\frac{1}{2}$	1	−1	1				1	2
$\frac{1}{2}\eta\frac{1}{2}$	−1	−1	1				4	1
00ζ	1	1	1				4	1
$\frac{1}{2}0\zeta$	−1	1	−1				1	2
$0\frac{1}{2}\zeta$	1	−1	1				1	2
$\frac{1}{2}\frac{1}{2}\zeta$	−1	−1	−1				1	2
$0\eta\zeta$	1						2	1
$\frac{1}{2}\eta\zeta$	−1						2	1
$\xi 0\zeta$	1						2	1
$\xi\frac{1}{2}\zeta$	−1						2	1
$\xi\eta 0$	1						2	1
$\xi\eta\frac{1}{2}$	−1						2	1
$\xi\eta\zeta$							1	1

For the subgroups, the defining relations follow from these. The corresponding expressions in the representation matrices $\Gamma(A_i)$ for the generators of the point groups give expressions

$$W_i^{\rm left}(A_1, \ldots, A_r) = \lambda_i W_i^{\rm right}(A_1, \ldots, A_r), \quad i = 1, \ldots.$$

In the example one has

$$\begin{array}{ll} \Gamma(A)^2 = \lambda_1 E & \Gamma(B)^2 = \lambda_2 E \\ (\Gamma(A)\Gamma(B))^2 = \lambda_3 E & \Gamma(C)^2 = \lambda_4 E \\ \Gamma(A)\Gamma(C) = \lambda_5 \Gamma(C)\Gamma(A) & \Gamma(B)\Gamma(C) = \lambda_6 \Gamma(C)\Gamma(B). \end{array}$$

The values for λ_i characterize the projective representation factor system and are given in Table 1.2.3.3. They are unity for ordinary representations.

By putting factors i in front of the representation matrices in the appropriate places, some of the values of λ_i can be changed from -1 to $+1$. In this way, one obtains either ordinary representations, which are necessarily one-dimensional for these Abelian groups, or projective representations, which are in this case two-dimensional. This is indicated as well in Table 1.2.3.3. The one-dimensional irreducible representations are ordinary representations of the group $K_{\mathbf{k}}$. The two-dimensional ones are projective representations, but correspond to ordinary representations of the larger groups isomorphic to $D_4 \times C_2$ and D_4.

1.2.3.5. *Double space groups and their representations*

In Section 1.2.2.9, it was mentioned that the transformation properties of spin-$\frac{1}{2}$ particles under rotations are not given by the orthogonal group $O(3)$, but by the covering group $SU(2)$. Hence, the transformation of a spinor field under a Euclidean transformation g is given by

$$g\Psi(\mathbf{r}) = \pm U(R)\Psi(R^{-1}(\mathbf{r} - \mathbf{a})) \quad \forall\ g = \{R|\mathbf{a}\} \in E(3), \quad (1.2.3.27)$$

where the $SU(2)$ operator $U(R)$ is given by

$$U(R) = E\cos(\varphi/2) + (\boldsymbol{\sigma} \cdot \mathbf{n})\sin(\varphi/2) \quad (1.2.3.28)$$

when the rotation R has angle φ and axis $\mathbf{n}$. When R does not belong to $SO(3)$ one has to take $U(-R)$.

For an ordinary space group, one can construct the double space group by

$$\{R|\mathbf{a}\} \rightarrow \{\pm U(R)|\mathbf{a}\} \quad (1.2.3.29)$$

with multiplication rule

$$\{U(R)|\mathbf{a}\}\{U(S)|\mathbf{b}\} = \{U(R)U(S)|\mathbf{a} + R\mathbf{b}\}. \quad (1.2.3.30)$$

An invariant subgroup of the double space group is the translation group A. The factor group is the double point group K^d of the point group K.

The representations of the double space groups can be constructed in the same way as those of ordinary space groups. They are characterized by a vector $\mathbf{k}$ in the Brillouin zone and a label for an irreducible, generally projective, representation of the (double) point group $K^d_{\mathbf{k}}$ of $\mathbf{k}$, which is the double group of $K_{\mathbf{k}}$. Again, for nonsymmorphic space groups or wavevectors $\mathbf{k}$ inside the Brillouin zone, the relevant irreducible representations of $K^d_{\mathbf{k}}$ are ordinary representations with a trivial factor system.

For an element g of the space group G, there are two elements of the double space group G^d. If one considers an irreducible representation $D(G^d)$ for the double space group and takes for each $g \in G$ one of the two corresponding elements in G^d, the resulting set of linear operators forms a projective representation of the space group. It is also characterized by a vector $\mathbf{k}$ in the Brillouin zone and a projective representation of the point group (not its double) $K_{\mathbf{k}}$. This projective representation does not have the same factor system as discussed in Section 1.2.3.3, because the factor system now stems partly from the nonprimitive translations and partly from the fact that a double point group gives a projective representation of the ordinary point group $K_{\mathbf{k}}$.

The projective representations of a space group corresponding to ordinary representations of the double space group again are characterized by the star of a vector $\mathbf{k}$. The projective representation of the group $G_{\mathbf{k}}$ then is given by

$$P_{\mathbf{k}}(\{R|\mathbf{a}\}) = \exp(i\mathbf{k} \cdot \mathbf{a})\Gamma(R), \quad (1.2.3.31)$$

where the projective representation $\Gamma(K_{\mathbf{k}})$ has the factor system

$$\begin{aligned} \Gamma(R)\Gamma(S) &= \omega_s(R, S)\exp[-i(\mathbf{k} - R^{-1}\mathbf{k}) \cdot \mathbf{a}(S)]\Gamma(RS) \\ &= \omega(R, S)\Gamma(RS), \end{aligned} \quad (1.2.3.32)$$

where ω_s is the spin factor system for $K_{\mathbf{k}}$ and $\mathbf{a}(S)$ is the nonprimitive translation of the space-group element with orthogonal part S. The factor system ω can be characterized by the defining relations of $K_{\mathbf{k}}$. If these are the words

$$W_i(A_1, \ldots, A_p) = E,$$

then the factor system ω is characterized by the factors λ_i in

$$W_i(\Gamma(A_1), \ldots, \Gamma(A_p)) = \lambda_i E. \quad (1.2.3.33)$$

The factors λ_i are the product of the values found from the spin factor system ω_s and those corresponding to the factor system for an ordinary representation [equation (1.2.3.26)].

1.2.4. Tensors

1.2.4.1. *Transformation properties of tensors*

A vector is an element of an N-dimensional vector space that transforms under an orthogonal transformation, an element of $O(n)$, as

$$x = \sum_{i=1}^{n} \xi_i \mathbf{a}_i \rightarrow x' = \sum_{i=1}^{n} \xi_i' \mathbf{a}_i = \sum_{ij} R_{ij} \xi_j \mathbf{a}_i, \quad \{R_{ij}\} \in O(n).$$

A tensor of rank r under $O(n)$ is an object with components $T_{i_1 \ldots i_r}$ ($i_j = 1, 2, \ldots, n$) that transforms as (see Section 1.1.3.2)

$$T_{i_1 \ldots i_r} \rightarrow T'_{i_1 \ldots i_r} = \sum_{j_1=1}^{n} \ldots \sum_{j_r=1}^{n} R_{i_1 j_1} \ldots R_{i_r j_r} T_{j_1 \ldots j_r}.$$

A rank-zero tensor is a scalar, which is invariant under $O(n)$. A pseudovector (or axial vector) has components x_i and transforms according to

$$x_i \rightarrow x_i' = \mathrm{Det}(R) \sum_j R_{ij} \xi_j$$

and analogously for pseudotensors (or axial tensors – see Section 1.1.4.5.3).

A vector field is a vector-valued function in n-dimensional space. Under an orthogonal transformation it transforms according to

$$F_i(\mathbf{r})' = \sum_{j=1}^{n} R_{ij} F_j(R^{-1}\mathbf{r}). \qquad (1.2.4.1)$$

Under a Euclidean transformation, the function transforms according to

$$F_i(\mathbf{r})' = \sum_{j=1}^{n} R_{ij} F_j(R^{-1}(\mathbf{r} - \mathbf{a})), \quad \{R|\mathbf{a}\} \in E(n). \qquad (1.2.4.2)$$

In a similar way, one has (pseudo)tensor functions under the orthogonal group or the Euclidean group. So it is important to specify under what group an object is a tensor, unless no confusion is possible.

The n-dimensional vectors form a vector space that carries a representation of the group $O(n)$. Moreover, it is an irreducible representation space. To stress this fact, one could speak of *irreducible tensors and vectors*. Vectors are here just rank-one tensors. The three-dimensional Euclidean vector space carries in this way an irreducible representation of $O(3)$. Such representations are characterized by an integer l and are $(2l+1)$-dimensional. The usual three-dimensional space is therefore an irreducible $l = 1$ space for $O(3)$.

Since point groups are subgroups of the orthogonal group and space groups are subgroups of the Euclidean group, tensors inherit their transformation properties from their supergroups. As we have seen in Sections 1.2.2.3 and 1.2.2.7, one can also define tensors in a quite abstract way. Irreducible tensors under a group are then elements of a vector space that carries an irreducible representation of that group. Generally, tensors are elements of a vector space that carries a tensor product representation and (anti)symmetric tensors belong to a space with an (anti)symmetrized tensor product representation.

Because the point groups one usually considers in physics are subgroups of $O(2)$ or $O(3)$, it is useful to consider the irreducible representations of these groups. The groups $O(2)$ and $O(3)$ are not finite, but they are compact, and for compact groups most of the theorems for finite groups are still valid if one replaces sums over group elements by integration over the group.

The group $O(3)$ is the direct product $SO(3) \times C_2$. Therefore, there are even and odd representations. They have the property

$$D^{\pm}(R) = \Delta(R), \quad D^{\pm}(-R) = \pm\Delta(R), \quad R \in SO(3).$$

The irreducible representations are labelled by non-negative integers ℓ and have character

$$\chi_\ell(R) = \frac{\sin(\ell + \frac{1}{2})\varphi}{\sin \frac{1}{2}\varphi} \qquad (1.2.4.3)$$

if R is a rotation with rotation angle φ. From the character it follows that the dimension of the representation D_ℓ is equal to $(2\ell + 1)$.

The tensor product of two irreducible representations of $SO(3)$ is generally reducible:

$$D_\ell \otimes D_m = \bigoplus_{j=|\ell-m|}^{\ell+m} D_j \qquad (1.2.4.4)$$

and the symmetrized and antisymmetrized tensor products are

$$(D_m \otimes D_m)_s = \bigoplus_{j=0}^{m} D_{2j}, \qquad (1.2.4.5)$$

$$(D_m \otimes D_m)_a = \bigoplus_{j=1}^{m} D_{2j-1}. \qquad (1.2.4.6)$$

If the components of the tensor $T_{i_1 \ldots i_r}$ are taken with respect to an orthonormal basis, the tensor is called a *Cartesian tensor*. The orthogonal transformation R then is represented by an orthogonal matrix R_{ij}. Cartesian tensors of higher rank than one are generally no longer irreducible for the group $O(n)$. For example, the rank-two tensors in three dimensions have nine components T_{ij}. Under $SO(3)$, they transform according to the tensor product of two $\ell = 1$ representations. Because

$$D_1 \otimes D_1 = D_0 \oplus D_1 \oplus D_2,$$

the space of rank 2 Cartesian tensors is the direct sum of three invariant subspaces. This corresponds to the fact that a general rank 2 tensor can be written as the sum of a diagonal tensor, an antisymmetric tensor and a symmetric tensor with trace zero. These three tensors are irreducible tensors, in this case also called *spherical tensors*, *i.e.* irreducible tensors for the orthogonal group.

An irreducible tensor with respect to the group $O(3)$ transforms, in general, according to some reducible representation of a point group $K \in O(3)$. If the group K is a symmetry of the physical system, the tensor should be invariant under K, *i.e.* it should transform according to the identity representation of K.

Consider, for example, a symmetric second-rank tensor under $O(3)$. This means that it belongs to the space that transforms according to the representation

$$D_0 \oplus D_2$$

[see (1.2.4.6)]. If the symmetry group of the system is the point group $K = 432$, the representation

$$D_0(K) \oplus D_2(K)$$

has character

R:	ε	$\beta = C_3$	$\alpha^2 = C_{4z}^2$	$\alpha = C_{4z}$	$\alpha\beta = C_2$
$\chi(R)$:	6	0	2	0	2

and is equivalent to the direct sum