Definition

Let $\mathbf{L}$ be a three-dimensional lattice with metric tensor $\boldsymbol{G}$ with respect to a primitive basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$.

(i) An *automorphism* of $\mathbf{L}$ is an isometry mapping $\mathbf{L}$ to itself. Written with respect to the basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$, an automorphism of $\mathbf{L}$ is an integral basis transformation fixing the metric tensor of $\mathbf{L}$, *i.e.* it is an integral matrix $\boldsymbol{W} \in \mathrm{GL}_3(\mathbb{Z})$ with $\boldsymbol{W}^{\mathrm{T}} \cdot \boldsymbol{G} \cdot \boldsymbol{W} = \boldsymbol{G}$.

(ii) The group

$$\mathcal{B} := Aut(\mathbf{L}) = \{\boldsymbol{W} \in \mathrm{GL}_3(\mathbb{Z}) \mid \boldsymbol{W}^{\mathrm{T}} \cdot \boldsymbol{G} \cdot \boldsymbol{W} = \boldsymbol{G}\}$$

of all automorphisms of $\mathbf{L}$ is called the *automorphism group* or *Bravais group* of $\mathbf{L}$. Note that $Aut(\mathbf{L})$ acts on the coordinate columns of $\mathbf{L}$, which are simply columns with integral coordinates.

Since the isometries in the Bravais group of a lattice preserve distances, the possible images of the vectors in a basis are vectors of the same lengths as the basis vectors. But due to its discreteness, a lattice contains only finitely many lattice vectors up to a given length. This means that a lattice automorphism can only permute the finitely many vectors up to the maximum length of a basis vector. Thus, there can only be finitely many automorphisms of a lattice. This argument proves the following important fact:

Theorem. The Bravais group of a lattice is finite. As a consequence, point groups of space groups are finite groups.

As subgroups of the Bravais group of a lattice, point groups can be realized as integral matrix groups when written with respect to a primitive basis. For a centred lattice, it is possible that the Bravais group of a lattice contains non-integral matrices, because the centring vector is a column with non-integral entries. However, in dimensions two and three the conventional bases are chosen such that the Bravais groups of all lattices are integral when written with respect to a conventional basis.

Information on the Bravais groups of the primitive lattices in two- and three-dimensional space is displayed in Tables 1.3.3.1 and 1.3.3.2. The columns of the tables contain the names of the lattices, the metric tensor with respect to the conventional basis (with only the upper half given, the lower half following by the symmetry of the metric tensor), the Hermann–Mauguin symbol for the type of the Bravais group and generators of the Bravais group (given in the shorthand notation introduced in Section 1.2.2.1 and the corresponding Seitz symbols discussed in Section 1.4.2.2).

The finiteness and integrality of the point groups has important consequences. For example, it implies the *crystallographic restriction* that rotations in space groups of two- and three-dimensional space can only have orders 1, 2, 3, 4 or 6. On the one hand, an integral matrix clearly has an integral trace.[1] But a matrix $\boldsymbol{W}$ with the property that $\boldsymbol{W}^k = \boldsymbol{I}$ can be diagonalized over the complex numbers and the diagonal entries have to be kth roots of unity, *i.e.* powers of $\zeta_k = \exp(2\pi i/k)$. Since diagonalization does not change the trace, the sum of these kth roots of unity still has to be an integer and in particular these roots of unity have to occur in complex conjugate pairs. In dimension 2 this means that the two diagonal entries are complex conjugate and the only possible ways to obtain an integral trace are $\zeta_1 + \zeta_1^{-1} = 2$, $\zeta_2 + \zeta_2^{-1} = -2$, $\zeta_3 + \zeta_3^{-1} = -1$, $\zeta_4 + \zeta_4^{-1} = 0$ and $\zeta_6 + \zeta_6^{-1} = 1$. In dimension 3 the third diagonal entry does not have a complex conjugate partner, and therefore has to be ± 1.

[1] The trace of a matrix is the sum of its diagonal entries.

Table 1.3.3.1
Automorphism groups of two-dimensional primitive lattices

Lattice	Metric tensor	Bravais group	
		Hermann–Mauguin symbol	Generators
Oblique	$\begin{pmatrix} g_{11} & g_{12} \\ & g_{22} \end{pmatrix}$	2	2: $\bar{x}, \bar{y}$
Rectangular	$\begin{pmatrix} g_{11} & 0 \\ & g_{22} \end{pmatrix}$	$2mm$	2: $\bar{x}, \bar{y}$ m_{10}: $\bar{x}, y$
Square	$\begin{pmatrix} g_{11} & 0 \\ & g_{11} \end{pmatrix}$	$4mm$	4^+: $\bar{y}, x$ m_{10}: $\bar{x}, y$
Hexagonal	$\begin{pmatrix} g_{11} & -\frac{1}{2}g_{11} \\ & g_{11} \end{pmatrix}$	$6mm$	6^+: $x - y, x$ m_{21}: $\bar{x}, \bar{x} + y$

Thus the possible orders in dimension 3 are the same as in dimension 2.

A much stronger result was obtained by H. Minkowski (1887). He gave an explicit bound for the maximal power p^m of a prime p which can divide the order of an n-dimensional finite integral matrix group. In dimension 2 this theorem implies that the orders of the point groups divide 24 and in dimension 3 the orders of the point groups divide 48. The Bravais groups $4mm$ (of order 8) and $6mm$ (of order 12) of the square and hexagonal lattices in dimension 2 and the Bravais group $m\bar{3}m$ (of order 48) of the cubic lattice in dimension 3 show that Minkowski's result is the best possible in these dimensions.

1.3.3.2. Coset decomposition with respect to the translation subgroup

The translation subgroup $\mathcal{T}$ of a space group $\mathcal{G}$ can be used to distribute the operations of $\mathcal{G}$ into different classes by grouping together all operations that differ only by a translation. This results in the decomposition of $\mathcal{G}$ into cosets with respect to $\mathcal{T}$ (see Section 1.1.4 for details of cosets).

Definition

Let $\mathcal{G}$ be a space group with translation subgroup $\mathcal{T}$.

(i) The *right coset* $\mathcal{T}W$ of an operation $W \in \mathcal{G}$ with respect to $\mathcal{T}$ is the set $\{tW \mid t \in \mathcal{T}\}$.
Analogously, the set $W\mathcal{T} = \{Wt \mid t \in \mathcal{T}\}$ is called the *left coset* of W with respect to $\mathcal{T}$.

(ii) A set $\{W_1, \ldots, W_m\}$ of operations in $\mathcal{G}$ is called a system of *coset representatives* relative to $\mathcal{T}$ if every operation W in $\mathcal{G}$ is contained in exactly one coset $\mathcal{T}W_i$.

(iii) Writing $\mathcal{G}$ as the disjoint union

$$\mathcal{G} = \mathcal{T}W_1 \cup \ldots \cup \mathcal{T}W_m$$

is called the *coset decomposition of* $\mathcal{G}$ *relative to* $\mathcal{T}$.

If the translation subgroup $\mathcal{T}$ is a subgroup of index $[i]$ in $\mathcal{G}$, a set of coset representatives for $\mathcal{G}$ relative to $\mathcal{T}$ consists of $[i]$ operations $W_1, W_2, \ldots, W_{[i]}$, where W_1 is assumed to be the identity element e of $\mathcal{G}$. The cosets of $\mathcal{G}$ relative to $\mathcal{T}$ can be imagined as columns of an infinite array with $[i]$ columns, labelled by the coset representatives, as displayed in Table 1.3.3.3.

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