International Tables for Crystallography (2006). Vol. B, Section 1.3.4.2.2.2, pp. 64–66.

This formula played an important role in the solution of the 2D Ising model by Onsager (1944) (see Montroll *et al.*, 1963). It is also encountered in phasing methods involving the 'Burg entropy' (Britten & Collins, 1982; Narayan & Nityananda, 1982; Bricogne, 1982, 1984, 1988).

1.3.4.2.2. *Crystal symmetry*

1.3.4.2.2.1. *Crystallographic groups*

The description of a crystal given so far has dealt only with its invariance under the action of the (discrete Abelian) group of translations by vectors of its period lattice Λ.

Let the crystal now be embedded in Euclidean 3-space, so that it may be acted upon by the group $M(3)$ of rigid (*i.e.* distance-preserving) motions of that space. The group $M(3)$ contains a normal subgroup $T(3)$ of translations, and the quotient group $M(3)/T(3)$ may be identified with the 3-dimensional orthogonal group $O(3)$. The period lattice Λ of a crystal is a discrete uniform subgroup of $T(3)$.

The possible invariance properties of a crystal under the action of $M(3)$ are captured by the following definition: a *crystallographic group* is a subgroup Γ of $M(3)$ if

(i) $\Gamma \cap T(3) = \Lambda$, a period lattice and a normal subgroup of Γ;

(ii) the factor group $G = \Gamma/\Lambda$ is finite.

The two properties are not independent: by a theorem of Bieberbach (1911), they follow from the assumption that Λ is a discrete subgroup of $M(3)$ which operates without accumulation point and with a compact fundamental domain (see Auslander, 1965). These two assumptions imply that G acts on Λ through an integral representation, and this observation leads to a complete enumeration of all distinct Γ's. The mathematical theory of these groups is still an active research topic (see, for instance, Farkas, 1981), and has applications to Riemannian geometry (Wolf, 1967).

This classification of crystallographic groups is described elsewhere in these *Tables* (Wondratschek, 1995), but it will be surveyed briefly in Section 1.3.4.2.2.3 for the purpose of establishing further terminology and notation, after recalling basic notions and results concerning groups and group actions in Section 1.3.4.2.2.2.

1.3.4.2.2.2. *Groups and group actions*

The books by Hall (1959) and Scott (1964) are recommended as reference works on group theory.

(*a*) *Left and right actions*

Let G be a group with identity element e, and let X be a set. An *action* of G on X is a mapping from $G \times X$ to X with the property that, if $g\,x$ denotes the image of (g, x), then

(i) $(g_1 g_2)x = g_1(g_2 x)$ for all $g_1, g_2 \in G$ and all $x \in X$,

(ii) $ex = x$ for all $x \in X$.

An element g of G thus induces a mapping T_g of X into itself defined by $T_g(x) = gx$, with the 'representation property':

(iii) $T_{g_1 g_2} = T_{g_1} T_{g_2}$ for all $g_1, g_2 \in G$.

Since G is a group, every g has an inverse g^{-1}; hence every mapping T_g has an inverse $T_{g^{-1}}$, so that each T_g is a permutation of X.

Strictly speaking, what has just been defined is a *left* action. A *right* action of G on X is defined similarly as a mapping $(g, x) \longmapsto xg$ such that

(i′) $x(g_1 g_2) = (xg_1)g_2$ for all $g_1, g_2 \in G$ and all $x \in X$,

(ii′) $xe = x$ for all $x \in X$.

The mapping T'_g defined by $T'_g(x) = xg$ then has the 'right-representation' property:

(iii′) $T'_{g_1 g_2} = T'_{g_2} T'_{g_1}$ for all $g_1, g_2 \in G$.

The essential difference between left and right actions is of course not whether the elements of G are written on the left or right of those of X: it lies in the difference between (iii) and (iii′). In a left action the product $g_1 g_2$ in G operates on $x \in X$ by g_2 operating first, then g_1 operating on the result; in a right action, g_1 operates first, then g_2. This distinction will be of importance in Sections 1.3.4.2.2.4 and 1.3.4.2.2.5. In the sequel, we will use left actions unless otherwise stated.

(*b*) *Orbits and isotropy subgroups*

Let x be a fixed element of X. Two fundamental entities are associated to x:

(1) the subset of G consisting of all g such that $gx = x$ is a subgroup of G, called the *isotropy subgroup* of x and denoted G_x;

(2) the subset of X consisting of all elements gx with g running through G is called the *orbit* of x under G and is denoted Gx.

Through these definitions, the action of G on X can be related to the internal structure of G, as follows. Let G/G_x denote the collection of distinct left cosets of G_x in G, *i.e.* of distinct subsets of G of the form gG_x. Let $|G|, |G_x|, |Gx|$ and $|G/G_x|$ denote the numbers of elements in the corresponding sets. The number $|G/G_x|$ of distinct cosets of G_x in G is also denoted $[G : G_x]$ and is called the *index* of G_x in G; by Lagrange's theorem

$$[G : G_x] = |G/G_x| = \frac{|G|}{|G_x|}.$$

Now if g_1 and g_2 are in the same coset of G_x, then $g_2 = g_1 g'$ with $g' \in G_x$, and hence $g_1 x = g_2 x$; the converse is obviously true. Therefore, the mapping from cosets to orbit elements

$$gG_x \longmapsto gx$$

establishes a one-to-one correspondence between the distinct left cosets of G_x in G and the elements of the orbit of x under G. It follows that the number of distinct elements in the orbit of x is equal to the index of G_x in G:

$$|Gx| = [G : G_x] = \frac{|G|}{|G_x|},$$

and that the elements of the orbit of x may be listed without repetition in the form

$$Gx = \{\gamma x | \gamma \in G/G_x\}.$$

Similar definitions may be given for a right action of G on X. The set of distinct right cosets $G_x g$ in G, denoted $G_x \backslash G$, is then in one-to-one correspondence with the distinct elements in the orbit xG of x.

(*c*) *Fundamental domain and orbit decomposition*

The group properties of G imply that two orbits under G are either disjoint or equal. The set X may thus be written as the *disjoint* union

$$X = \bigcup_{i \in I} Gx_i,$$

where the x_i are elements of distinct orbits and I is an indexing set labelling them. The subset $D = \{x_i\}_{i \in I}$ is said to constitute a *fundamental domain* (mathematical terminology) or an *asymmetric unit* (crystallographic terminology) for the action of G on X: it contains one representative x_i of each distinct orbit. Clearly, other fundamental domains may be obtained by choosing different representatives for these orbits.

If X is finite and if f is an arbitrary complex-valued function over X, the 'integral' of f over X may be written as a sum of integrals over the distinct orbits, yielding the *orbit decomposition formula*:

$$\sum_{x \in X} f(x) = \sum_{i \in I} \left(\sum_{y_i \in Gx_i} f(y_i) \right) = \sum_{i \in I} \left(\sum_{\gamma_i \in G/G_{x_i}} f(\gamma_i x_i) \right)$$
$$= \sum_{i \in I} \frac{1}{|G_{x_i}|} \left(\sum_{g_i \in G} f(g_i x_i) \right).$$

In particular, taking $f(x) = 1$ for all x and denoting by $|X|$ the number of elements of X:

$$|X| = \sum_{i \in I} |Gx_i| = \sum_{i \in I} |G/G_{x_i}| = \sum_{i \in I} \frac{|G|}{|G_{x_i}|}.$$

(*d*) *Conjugation, normal subgroups, semi-direct products*

A group G acts on itself by *conjugation*, *i.e.* by associating to $g \in G$ the mapping C_g defined by

$$C_g(h) = ghg^{-1}.$$

Indeed, $C_g(hk) = C_g(h)C_g(k)$ and $[C_g(h)]^{-1} = C_{g^{-1}}(h)$. In particular, C_g operates on the set of subgroups of G, two subgroups H and K being called conjugate if $H = C_g(K)$ for some $g \in G$; for example, it is easily checked that $G_{gx} = C_g(G_x)$. The orbits under this action are the *conjugacy classes* of subgroups of G, and the isotropy subgroup of H under this action is called the *normalizer* of H in G.

If $\{H\}$ is a one-element orbit, H is called a *self-conjugate* or *normal* subgroup of G; the cosets of H in G then form a group G/H called the *factor group* of G by H.

Let G and H be two groups, and suppose that G acts on H by *automorphisms* of H, *i.e.* in such a way that

$$g(h_1 h_2) = g(h_1) g(h_2)$$
$$g(e_H) = e_H \qquad \text{(where } e_H \text{ is the identity element of } H).$$
$$g(h^{-1}) = (g(h))^{-1}$$

Then the symbols $[g, h]$ with $g \in G, h \in H$ form a group K under the product rule:

$$[g_1, h_1][g_2, h_2] = [g_1 g_2, h_1 g_1(h_2)]$$

{associativity checks; $[e_G, e_H]$ is the identity; $[g, h]$ has inverse $[g^{-1}, g^{-1}(h^{-1})]$}. The group K is called the *semi-direct product* of H by G, denoted $K = H \rtimes G$.

The elements $[g, e_H]$ form a subgroup of K isomorphic to G, the elements $[e_G, h]$ form a normal subgroup of K isomorphic to H, and the action of G on H may be represented as an action by conjugation in the sense that

$$C_{[g,\, e_H]}([e_G, h]) = [e_G, g(h)].$$

A familiar example of semi-direct product is provided by the group of Euclidean motions $M(3)$ (Section 1.3.4.2.2.1). An element S of $M(3)$ may be written $S = [R, t]$ with $R \in O(3)$, the orthogonal group, and $t \in T(3)$, the translation group, and the product law

$$[R_1, t_1][R_2, t_2] = [R_1 R_2, t_1 + R_1(t_2)]$$

shows that $M(3) = T(3) \rtimes O(3)$ with $O(3)$ acting on $T(3)$ by rotating the translation vectors.

(*e*) *Associated actions in function spaces*

For every left action T_g of G in X, there is an associated left action $T_g^\#$ of G on the space $L(X)$ of complex-valued functions over X, defined by 'change of variable' (Section 1.3.2.3.9.5):

$$[T_g^\# f](x) = f((T_g)^{-1} x) = f(g^{-1} x).$$

Indeed for any g_1, g_2 in G,

$$[T_{g_1}^\# [T_{g_2}^\# f]](x) = [T_{g_2}^\# f]((T_{g_1})^{-1} x) = f[T_{g_2}^{-1} T_{g_1}^{-1} x]$$
$$= f((T_{g_1} T_{g_2})^{-1} x);$$

since $T_{g_1} T_{g_2} = T_{g_1 g_2}$, it follows that

$$T_{g_1}^\# T_{g_2}^\# = T_{g_1 g_2}^\#.$$

It is clear that the change of variable must involve the action of g^{-1} (not g) if $T^\#$ is to define a *left* action; using g instead would yield a *right* action.

The linear representation operators $T_g^\#$ on $L(X)$ provide the most natural instrument for stating and exploiting symmetry properties which a function may possess with respect to the action of G. Thus a function $f \in L(X)$ will be called *G-invariant* if $f(gx) = f(x)$ for all $g \in G$ and all $x \in X$. The value $f(x)$ then depends on x only through its orbit Gx, and f is uniquely defined once it is specified on a fundamental domain $D = \{x_i\}_{i \in I}$; its integral over X is then a weighted sum of its values in D:

$$\sum_{x \in X} f(x) = \sum_{i \in I} [G : G_{x_i}] f(x_i).$$

The G-invariance of f may be written:

$$T_g^\# f = f \quad \text{for all } g \in G.$$

Thus f is invariant under each $T_g^\#$, which obviously implies that f is invariant under the linear operator in $L(X)$

$$A_G = \frac{1}{|G|} \sum_{g \in G} T_g^\#,$$

which averages an arbitrary function by the action of G. Conversely, if $A_G f = f$, then

$$T_{g_0}^\# f = T_{g_0}^\# (A_G f) = (T_{g_0}^\# A_G) f = A_G f = f \quad \text{for all } g_0 \in G,$$

so that the two statements of the G-invariance of f are equivalent. The identity

$$T_{g_0}^\# A_G = A_G \quad \text{for all } g_0 \in G$$

is easily proved by observing that the map $g \longmapsto g_0 g$ (g_0 being any element of G) is a one-to-one map from G into itself, so that

$$\sum_{g \in G} T_g^\# = \sum_{g \in G} T_{g_0 g}^\#$$

as these sums differ only by the order of the terms. The same identity implies that A_G is a *projector*:

$$(A_G)^2 = A_G,$$

and hence that its eigenvalues are either 0 or 1. In summary, we may say that the invariance of f under G is equivalent to f being an eigenfunction of the associated projector A_G for eigenvalue 1.

(*f*) *Orbit exchange*

One final result about group actions which will be used repeatedly later is concerned with the case when X has the structure of a Cartesian product:

$$X = X_1 \times X_2 \times \ldots \times X_n$$

and when G acts *diagonally* on X, *i.e.* acts on each X_j separately:

$$gx = g(x_1, x_2, \ldots, x_n) = (gx_1, gx_2, \ldots, gx_n).$$

Then complete sets (but not usually minimal sets) of representatives of the distinct orbits for the action of G in X may be obtained in the form

$$D_k = X_1 \times \ldots \times X_{k-1} \times \{x_{i_k}^{(k)}\}_{i_k \in I_k} \times X_{k+1} \times \ldots \times X_n$$

for each $k = 1, 2, \ldots, n$, *i.e.* by taking a fundamental domain in X_k and all the elements in X_j with $j \neq k$. The action of G on each D_k does indeed generate the whole of X: given an arbitrary element $y = (y_1, y_2, \ldots, y_n)$ of X, there is an index $i_k \in I_k$ such that $y_k \in Gx_{i_k}^{(k)}$ and a coset of $G_{x_{i_k}^{(k)}}$ in G such that $y_k = \gamma x_{i_k}^{(k)}$ for any representative γ of that coset; then

$$y = \gamma(\gamma^{-1}y_1, \ldots, \gamma^{-1}y_{k-1}, x_{i_k}^{(k)}, \gamma^{-1}y_{k+1}, \ldots, \gamma^{-1}y_n)$$

which is of the form $y = \gamma d_k$ with $d_k \in D_k$.

The various D_k are related in a simple manner by 'transposition' or 'orbit exchange' (the latter name is due to J. W. Cooley). For instance, D_j may be obtained from D_k ($j \neq k$) as follows: for each $y_j \in X_j$ there exists $g(y_j) \in G$ and $i_j(y_j) \in I_j$ such that $y_j = g(y_j)x_{i_j(y_j)}^{(j)}$; therefore

$$D_j = \bigcup_{y_j \in X_j} [g(y_j)]^{-1} D_k,$$

since the fundamental domain of X_k is thus expanded to the whole of X_k, while X_j is reduced to its fundamental domain. In other words: orbits are simultaneously collapsed in the jth factor and expanded in the kth.

When G operates without fixed points in each X_k (*i.e.* $G_{x_k} = \{e\}$ for all $x_k \in X_k$), then each D_k is a fundamental domain for the action of G in X. The existence of fixed points in some or all of the X_k complicates the situation in that for each k and each $x_k \in X_k$ such that $G_{x_k} \neq \{e\}$ the action of G/G_{x_k} on the other factors must be examined. Shenefelt (1988) has made a systematic study of orbit exchange for space group $P622$ and its subgroups.

Orbit exchange will be encountered, in a great diversity of forms, as the basic mechanism by which intermediate results may be rearranged between the successive stages of the computation of crystallographic Fourier transforms (Section 1.3.4.3).

1.3.4.2.2.3. *Classification of crystallographic groups*

Let Γ be a crystallographic group, Λ the normal subgroup of its lattice translations, and G the finite factor group Γ/Λ. Then G acts on Λ by conjugation [Section 1.3.4.2.2.2(*d*)] and this action, being a mapping of a lattice into itself, is representable by matrices with integer entries.

The classification of crystallographic groups proceeds from this observation in the following three steps:

Step 1: find all possible finite abstract groups G which can be represented by 3×3 integer matrices.

Step 2: for each such G find all its inequivalent representations by 3×3 integer matrices, equivalence being defined by a change of primitive lattice basis (*i.e.* conjugation by a 3×3 integer matrix with determinant ± 1).

Step 3: for each G and each equivalence class of integral representations of G, find all inequivalent extensions of the action of G from Λ to $T(3)$, equivalence being defined by an affine coordinate change [*i.e.* conjugation by an element of $A(3)$].

Step 1 leads to the following groups, listed in association with the crystal system to which they later give rise:

$\mathbb{Z}/2\mathbb{Z}$	monoclinic
$\mathbb{Z}/2\mathbb{Z} \oplus \mathbb{Z}/2\mathbb{Z}$	orthorhombic
$\mathbb{Z}/3\mathbb{Z}, (\mathbb{Z}/3\mathbb{Z}) \ltimes \{\alpha\}$	trigonal
$\mathbb{Z}/4\mathbb{Z}, (\mathbb{Z}/4\mathbb{Z}) \ltimes \{\alpha\}$	tetragonal
$\mathbb{Z}/6\mathbb{Z}, (\mathbb{Z}/6\mathbb{Z}) \ltimes \{\alpha\}$	hexagonal
$(\mathbb{Z}/2\mathbb{Z} \oplus \mathbb{Z}/2\mathbb{Z}) \ltimes \{S_3\}$	cubic

and the extension of these groups by a centre of inversion. In this list $\ltimes$ denotes a semi-direct product [Section 1.3.4.2.2.2(*d*)], α denotes the automorphism $g \longmapsto g^{-1}$, and S_3 (the group of permutations on three letters) operates by permuting the copies of $\mathbb{Z}/2\mathbb{Z}$ (using the subgroup A_3 of cyclic permutations gives the tetrahedral subsystem).

Step 2 leads to a list of 73 equivalence classes called *arithmetic classes* of representations $g \longmapsto \mathbf{R}_g$, where $\mathbf{R}_g$ is a 3×3 integer matrix, with $\mathbf{R}_{g_1 g_2} = \mathbf{R}_{g_1}\mathbf{R}_{g_2}$ and $\mathbf{R}_e = \mathbf{I}_3$. This enumeration is more familiar if equivalence is relaxed so as to allow conjugation by *rational* 3×3 matrices with determinant $\pm$ 1: this leads to the 32 crystal classes. The difference between an arithmetic class and its rational class resides in the choice of a lattice mode (P, $A/B/C$, I, F or R). Arithmetic classes always refer to a primitive lattice, but may use inequivalent integral representations for a given geometric symmetry element; while crystallographers prefer to change over to a non-primitive lattice, if necessary, in order to preserve the same integral representation for a given geometric symmetry element. The matrices $\mathbf{P}$ and $\mathbf{Q} = \mathbf{P}^{-1}$ describing the changes of basis between primitive and centred lattices are listed in Table 5.1 and illustrated in Figs. 5.3 to 5.9, pp. 76–79, of Volume A of *International Tables* (Arnold, 1995).

Step 3 gives rise to a system of congruences for the systems of non-primitive translations $\{\mathbf{t}_g\}_{g \in G}$ which may be associated to the matrices $\{\mathbf{R}_g\}_{g \in G}$ of a given arithmetic class, namely:

$$\mathbf{t}_{g_1 g_2} \equiv \mathbf{R}_{g_1}\mathbf{t}_{g_2} + \mathbf{t}_{g_1} \bmod \Lambda,$$

first derived by Frobenius (1911). If equivalence under the action of $A(3)$ is taken into account, 219 classes are found. If equivalence is defined with respect to the action of the subgroup $A^+(3)$ of $A(3)$ consisting only of transformations with determinant +1, then 230 classes called *space-group types* are obtained. In particular, associating to each of the 73 arithmetic classes a trivial set of non-primitive translations ($\mathbf{t}_g = \mathbf{0}$ for all $g \in G$) yields the 73 symmorphic space groups. This third step may also be treated as an abstract problem concerning group extensions, using cohomological methods [Ascher & Janner (1965); see Janssen (1973) for a summary]; the connection with Frobenius's approach, as generalized by Zassenhaus (1948), is examined in Ascher & Janner (1968).

The finiteness of the number of space-group types in dimension 3 was shown by Bieberbach (1912) to be the case in arbitrary dimension. The reader interested in N-dimensional space-group theory for $N > 3$ may consult Brown (1969), Brown *et al.* (1978), Schwarzenberger (1980), and Engel (1986). The standard reference for integral representation theory is Curtis & Reiner (1962).

All three-dimensional space groups G have the property of being *solvable*, *i.e.* that there exists a chain of subgroups

$$G = G_r > G_{r-1} > \ldots > G_1 > G_0 = \{e\},$$

where each G_{i-1} is a normal subgroup of G_1 and the factor group G_i/G_{i-1} is a *cyclic* group of some order m_i $(1 \leq i \leq r)$. This property may be established by inspection, or deduced from a famous theorem of Burnside [see Burnside (1911), pp. 322–323] according to which any group G such that $|G| = p^\alpha q^\beta$, with p and q distinct primes, is solvable; in the case at hand, $p = 2$ and $q = 3$.

references