International Tables for Crystallography (2006). Vol. B, Section 1.3.4.3.3, p. 73.

integers, which accommodates 2D crystallographic symmetries in a most powerful and pleasing fashion.

At each stage of the calculation, it is necessary to keep track of the definition of the asymmetric unit and of the symmetry properties of the numbers being manipulated. This requirement applies not only to the initial data and to the final results, where these are familiar; but also to all the intermediate quantities produced by partial transforms (on subsets of factors, or subsets of dimensions, or both), where they are less familiar. Here, the general formalism of transposition (or 'orbit exchange') described in Section 1.3.4.2.2.2 plays a central role.

1.3.4.3.3. *Interaction between symmetry and decomposition*

Suppose that the space-group action is reducible, *i.e.* that for each $g \in G$

$$\mathbf{R}_g = \begin{pmatrix} \mathbf{R}'_g & \mathbf{0} \\ \mathbf{0} & \mathbf{R}''_g \end{pmatrix}, \qquad \mathbf{t}_g = \begin{pmatrix} \mathbf{t}'_g \\ \mathbf{t}''_g \end{pmatrix};$$

by Schur's lemma, the decimation matrix must then be of the form $\mathbf{N} = \begin{pmatrix} \mathbf{N}' & \mathbf{0} \\ \mathbf{0} & \mathbf{N}'' \end{pmatrix}$ if it is to commute with all the $\mathbf{R}_g$.

Putting $\mathbf{x} = \begin{pmatrix} \mathbf{x}' \\ \mathbf{x}'' \end{pmatrix}$ and $\mathbf{h} = \begin{pmatrix} \mathbf{h}' \\ \mathbf{h}'' \end{pmatrix}$, we may define

$$S'_g(\mathbf{x}') = \mathbf{R}'_g\mathbf{x}' + \mathbf{t}'_g,$$
$$S''_g(\mathbf{x}'') = \mathbf{R}''_g\mathbf{x}'' + \mathbf{t}''_g,$$

and write $S_g = S'_g \oplus S''_g$ (direct sum) as a shorthand for $S_g(\mathbf{x}) = \begin{pmatrix} S'_g(\mathbf{x}') \\ S''_g(\mathbf{x}'') \end{pmatrix}$.

We may also define the representation operators $S'^{\#}_g$ and $S''^{\#}_g$ acting on functions of $\mathbf{x}'$ and $\mathbf{x}''$, respectively (as in Section 1.3.4.2.2.4), and the operators S'^{*}_g and S''^{*}_g acting on functions of $\mathbf{h}'$ and $\mathbf{h}''$, respectively (as in Section 1.3.4.2.2.5). Then we may write

$$S^{\#}_g = (S'_g)^{\#} \oplus (S''_g)^{\#}$$

and

$$S^{*}_g = (S'_g)^{*} \oplus (S''_g)^{*}$$

in the sense that g acts on $f(\mathbf{x}) \equiv f(\mathbf{x}', \mathbf{x}'')$ by

$$(S^{\#}_g f)(\mathbf{x}', \mathbf{x}'') = f[(S'_g)^{-1}(\mathbf{x}'), (S''_g)^{-1}(\mathbf{x}'')]$$

and on $\Phi(\mathbf{h}) \equiv \Phi(\mathbf{h}', \mathbf{h}'')$ by

$$(S^{*}_g\Phi)(\mathbf{h}', \mathbf{h}'') = \exp(2\pi i\mathbf{h}' \cdot \mathbf{t}'_g)\exp(2\pi i\mathbf{h}'' \cdot \mathbf{t}''_g) \times \Phi[\mathbf{R}'^{T}_g\mathbf{h}', \mathbf{R}''^{T}_g\mathbf{h}''].$$

Thus equipped we may now derive concisely a general identity describing the symmetry properties of intermediate quantities of the form

$$T(\mathbf{x}', \mathbf{h}'') = \sum_{\mathbf{h}'} F(\mathbf{h}', \mathbf{h}'')\exp(-2\pi i\mathbf{h}' \cdot \mathbf{x}') = \frac{1}{|\det \mathbf{N}'|}\sum_{\mathbf{x}''} \rho(\mathbf{x}', \mathbf{x}'')\exp(+2\pi i\mathbf{h}'' \cdot \mathbf{x}''),$$

which arise through partial transformation of F on $\mathbf{h}'$ or of ρ on $\mathbf{x}''$. The action of $g \in G$ on these quantities will be

(i) through $(S'_g)^{\#}$ on the function $\mathbf{x}' \longmapsto T(\mathbf{x}', \mathbf{h}'')$,

(ii) through $(S''_g)^{*}$ on the function $\mathbf{h}'' \longmapsto T(\mathbf{x}', \mathbf{h}'')$,

and hence the symmetry properties of T are expressed by the identity

$$T = [(S'_g)^{\#} \oplus (S''_g)^{*}]T.$$

Applying this relation not to T but to $[(S'_{g^{-1}})^{\#} \oplus (S''_e)^{*}]T$ gives

$$[(S'_{g^{-1}})^{\#} \oplus (S''_e)^{*}]T = [(S'_e)^{\#} \oplus (S''_g)^{*}]T,$$

i.e.

$$\boxed{T(S'_g(\mathbf{x}'), \mathbf{h}'') = \exp(2\pi i\mathbf{h}'' \cdot \mathbf{t}''_g)T(\mathbf{x}', \mathbf{R}''^{T}_g\mathbf{h}'').}$$

If the unique $F(\mathbf{h}) \equiv F(\mathbf{h}', \mathbf{h}'')$ were initially indexed by

$$(\text{all } \mathbf{h}') \times (\text{unique } \mathbf{h}'')$$

(see Section 1.3.4.2.2.2), this formula allows the reindexing of the intermediate results $T(\mathbf{x}', \mathbf{h}'')$ from the initial form

$$(\text{all } \mathbf{x}') \times (\text{unique } \mathbf{h}'')$$

to the final form

$$(\text{unique } \mathbf{x}') \times (\text{all } \mathbf{h}''),$$

on which the second transform (on $\mathbf{h}''$) may now be performed, giving the final results $\rho(\mathbf{x}', \mathbf{x}'')$ indexed by

$$(\text{unique } \mathbf{x}') \times (\text{all } \mathbf{x}''),$$

which is an asymmetric unit. An analogous interpretation holds if one is going from ρ to F.

The above formula solves the general problem of transposing from one invariant subspace to another, and is the main device for decomposing the CDFT. Particular instances of this formula were derived and used by Ten Eyck (1973); it is useful for orthorhombic groups, and for dihedral groups containing screw axes n_m with g.c.d. $(m, n) = 1$. For comparison with later uses of orbit exchange, it should be noted that the type of intermediate results just dealt with is obtained after transforming on *all* factors in *one* summand.

A central piece of information for driving such a decomposition is the definition of the full asymmetric unit in terms of the asymmetric units in the invariant subspaces. As indicated at the end of Section 1.3.4.2.2.2, this is straightforward when G acts without fixed points, but becomes more involved if fixed points do exist. To this day, no systematic 'calculus of asymmetric units' exists which can automatically generate a complete description of the asymmetric unit of an arbitrary space group in a form suitable for directing the orbit exchange process, although Shenefelt (1988) has outlined a procedure for dealing with space group $P622$ and its subgroups. The asymmetric unit definitions given in Volume A of *International Tables* are incomplete in this respect, in that they do not specify the possible residual symmetries which may exist on the boundaries of the domains.

1.3.4.3.4. *Interaction between symmetry and factorization*

Methods for factoring the DFT in the absence of symmetry were examined in Sections 1.3.3.2 and 1.3.3.3. They are based on the observation that the finite sets which index both data and results are endowed with certain algebraic structures (*e.g.* are Abelian groups, or rings), and that subsets of indices may be found which are not merely subsets but *substructures* (*e.g.* subgroups or subrings). Summation over these substructures leads to partial transforms, and the way in which substructures fit into the global structure indicates how to reassemble the partial results into the final results. As a rule, the richer the algebraic structure which is identified in the indexing set, the more powerful the factoring method.

references