1.3.4.2.2.9. Convolution theorems with crystallographic symmetry

The standard convolution theorems derived in the absence of symmetry are readily seen to follow from simple properties of functions $e^{\pm}(\mathbf{h},\mathbf{x}) = \exp(\pm 2\pi i \mathbf{h}\cdot\mathbf{x})$ (denoted simply e in formulae which are valid for both signs), namely:

$$\text{(i)} \qquad e(\mathbf{h},\mathbf{x}) \times e(\mathbf{k},\mathbf{x}) = e(\mathbf{h}+\mathbf{k},\mathbf{x}),$$
$$\text{(ii)} \qquad e(\mathbf{h},\mathbf{x}) \times e(\mathbf{h},\mathbf{y}) = e(\mathbf{h},\mathbf{x}+\mathbf{y}).$$

These relations imply that the families of functions

$$\{\mathbf{x} \longmapsto e(\mathbf{h},\mathbf{x})\}_{\mathbf{h}\in\mathbb{Z}^3} \qquad \text{in real space}$$

and

$$\{\mathbf{h} \longmapsto e(\mathbf{h},\mathbf{x})\}_{\mathbf{x}\in\mathbb{R}^3/\mathbb{Z}^3} \qquad \text{in reciprocal space}$$

both generate an *algebra* of functions, *i.e.* a vector space endowed with an internal multiplication, since (i) and (ii) show how to 'linearize products'.

Friedel's law (when applicable) on the one hand, and the Fourier relation between intensities and the Patterson function on the other hand, both follow from the property

$$\text{(iii)} \qquad \overline{e(\mathbf{h},\mathbf{x})} = e(-\mathbf{h},\mathbf{x}) = e(\mathbf{h},-\mathbf{x}).$$

When crystallographic symmetry is present, the convolution theorems remain valid in their original form if written out in terms of 'expanded' data, but acquire a different form when rewritten in terms of symmetry-unique data only. This rewriting is made possible by the extra relation (Section 1.3.4.2.2.5)

$$\text{(iv)} \qquad S^{\#}_{g^{-1}} e(\mathbf{h},\mathbf{x}) \equiv e[\mathbf{h}, S_g(\mathbf{x})] = e(\mathbf{h},\mathbf{t}_g) e(\mathbf{R}_g^T\mathbf{h},\mathbf{x})$$

or equivalently

$$\text{(iv}') \qquad S^{\#}_{g} e(\mathbf{h},\mathbf{x}) \equiv e[\mathbf{h}, S_g^{-1}(\mathbf{x})] = e[(-\mathbf{R}_g^{-1})^T\mathbf{h},\mathbf{t}_g] e[(\mathbf{R}_g^{-1})^T\mathbf{h},\mathbf{x}].$$

The kernels of symmetrized Fourier transforms are not the functions e but rather the symmetrized sums

$$\Xi^{\pm}(\mathbf{h},\mathbf{x}) = \sum_{g\in G} e^{\pm}[\mathbf{h}, S_g(\mathbf{x})] = \sum_{g\in G} e^{\pm}[\mathbf{h}, S_g^{-1}(\mathbf{x})]$$

for which the linearization formulae are readily obtained using (i), (ii) and (iv) as

$$\text{(i)}_G \qquad \Xi^{\pm}(\mathbf{h},\mathbf{x})\Xi^{\pm}(\mathbf{k},\mathbf{x}) = \sum_{g\in G} e^{\pm}(\mathbf{k},\mathbf{t}_g)\Xi^{\pm}(\mathbf{h}+\mathbf{R}_g^T\mathbf{k},\mathbf{x}),$$
$$\text{(ii)}_G \qquad \Xi^{\pm}(\mathbf{h},\mathbf{x})\Xi^{\pm}(\mathbf{h},\mathbf{y}) = \sum_{g\in G} \Xi^{\pm}[\mathbf{h},\mathbf{x}+S_g(\mathbf{y})],$$

where the choice of sign in $\pm$ must be the same throughout each formula.

Formulae $(\text{i})_G$ defining the 'structure-factor algebra' associated to G were derived by Bertaut (1955*c*, 1956*b*,*c*, 1959*a*,*b*) and Bertaut & Waser (1957) in another context.

The forward convolution theorem (in discrete form) then follows. Let

$$F_1(\mathbf{h}) = \sum_{\mathbf{y}\in D} \frac{1}{|G_{\mathbf{y}}|} \rho_1(\mathbf{y}) \Xi^{+}(\mathbf{h},\mathbf{y}),$$
$$F_2(\mathbf{h}) = \sum_{\mathbf{z}\in D} \frac{1}{|G_{\mathbf{z}}|} \rho_2(\mathbf{z}) \Xi^{+}(\mathbf{h},\mathbf{z}),$$

then

$$F_1(\mathbf{h})F_2(\mathbf{h}) = \sum_{\mathbf{x}\in D} \frac{1}{|G_{\mathbf{x}}|} \sigma(\mathbf{x}) \Xi^{+}(\mathbf{h},\mathbf{x})$$

with

$$\sigma(\mathbf{x}) = \frac{1}{|\mathbf{N}|} \sum_{\mathbf{z}\in D} \sum_{g\in G} \frac{|G_{\mathbf{x}}|}{|G_{\mathbf{x}-S_g(\mathbf{z})}| \times |G_{\mathbf{z}}|} \rho_1[\mathbf{x}-S_g(\mathbf{z})]\rho_2(\mathbf{z}).$$

The backward convolution theorem is derived similarly. Let

$$\rho_1(\mathbf{x}) = \sum_{\mathbf{k}\in D^*} \frac{1}{|G_{\mathbf{k}}|} F_1(\mathbf{k}) \Xi^{-}(\mathbf{k},\mathbf{x}),$$
$$\rho_2(\mathbf{x}) = \sum_{\mathbf{l}\in D^*} \frac{1}{|G_{\mathbf{l}}|} F_2(\mathbf{l}) \Xi^{-}(\mathbf{l},\mathbf{x}),$$

then

$$\rho_1(\mathbf{x})\rho_2(\mathbf{x}) = \sum_{\mathbf{h}\in D^*} \frac{1}{|G_{\mathbf{h}}|} F(\mathbf{h}) \Xi^{-}(\mathbf{h},\mathbf{x})$$

with

$$F(\mathbf{h}) = \sum_{\mathbf{l}\in D^*} \sum_{g\in G} \frac{|G_{\mathbf{h}}|}{|G_{\mathbf{h}-\mathbf{R}_g^T(\mathbf{l})}| \times |G_{\mathbf{l}}|} e^{-}(\mathbf{l},\mathbf{t}_g) F_1(\mathbf{h}-\mathbf{R}_g^T\mathbf{l}) F_2(\mathbf{l}).$$

Both formulae are simply orbit decompositions of their symmetry-free counterparts.

1.3.4.2.2.10. Correlation and Patterson functions

Consider two model electron densities ρ_1 and ρ_2 with the same period lattice $\mathbb{Z}^3$ and the same space group G. Write their motifs in terms of atomic electron densities (Section 1.3.4.2.2.4) as

$$\rho_1^0 = \sum_{j_1\in J_1} \left(\sum_{\gamma_{j_1}\in G/G^{(1)}_{\mathbf{x}_{j_1}}} S^{\#}_{\gamma_{j_1}} (\tau_{\mathbf{x}^{(1)}_{j_1}} \rho^{(1)}_{j_1}) \right),$$
$$\rho_2^0 = \sum_{j_2\in J_2} \left(\sum_{\gamma_{j_2}\in G/G^{(2)}_{\mathbf{x}_{j_2}}} S^{\#}_{\gamma_{j_2}} (\tau_{\mathbf{x}^{(2)}_{j_2}} \rho^{(2)}_{j_2}) \right),$$

where J_1 and J_2 label the symmetry-unique atoms placed at positions $\{\mathbf{x}^{(1)}_{j_1}\}_{j_1\in J_1}$ and $\{\mathbf{x}^{(2)}_{j_2}\}_{j_2\in J_2}$, respectively.

To calculate the correlation between ρ_1 and ρ_2 we need the following preliminary formulae, which are easily established: if $S(\mathbf{x}) = \mathbf{R}\mathbf{x}+\mathbf{t}$ and f is an arbitrary function on $\mathbb{R}^3$, then

$$(R^{\#}f)\check{} = R^{\#}\check{f}, \quad (\tau_{\mathbf{x}} f)\check{} = \tau_{-\mathbf{x}}\check{f}, \quad R^{\#}(\tau_{\mathbf{x}} f) = \tau_{\mathbf{R}\mathbf{x}} f,$$

hence