International Tables for Crystallography (2006). Vol. B, Section 1.3.2.7.2.1, p. 46.

which is essentially Φ periodized by period lattice $\Lambda = (\Lambda^*)^*$, with period matrix **A**.

Let us assume that Λ is such that the translates of K by different period vectors of Λ are disjoint. Then we may recover Φ from $R * \Phi$ by masking the contents of a 'unit cell' $\mathscr{V}$ of Λ (*i.e.* a fundamental domain for the action of Λ in $\mathbb{R}^n$) whose boundary does not meet K. If $\chi_{\mathscr{V}}$ is the indicator function of $\mathscr{V}$, then

$$\Phi = \chi_{\mathscr{V}} \times (R * \Phi).$$

Transforming both sides by $\bar{\mathscr{F}}$ yields

$$\varphi = \bar{\mathscr{F}}\left[\chi_{\mathscr{V}} \times \frac{1}{|\det \mathbf{A}|}\mathscr{F}[R^* \times \varphi]\right],$$

i.e.

$$\varphi = \left(\frac{1}{V}\bar{\mathscr{F}}[\chi_{\mathscr{V}}]\right) * (R^* \times \varphi)$$

since $|\det \mathbf{A}|$ is the volume V of $\mathscr{V}$.

This interpolation formula is traditionally credited to Shannon (1949), although it was discovered much earlier by Whittaker (1915). It shows that φ may be recovered from its sample values on Λ^* (*i.e.* from $R^* \times \varphi$) provided Λ^* is sufficiently fine that no overlap (or 'aliasing') occurs in the periodization of Φ by the dual lattice Λ. The interpolation kernel is the transform of the normalized indicator function of a unit cell of Λ containing the support K of Φ.

If K is contained in a sphere of radius $1/\Delta$ and if Λ and Λ^* are rectangular, the length of each basis vector of Λ must be greater than $2/\Delta$, and thus the sampling interval must be smaller than $\Delta/2$. This requirement constitutes the Shannon sampling criterion.

1.3.2.7.2. *Duality between subdivision and decimation of period lattices*

1.3.2.7.2.1. *Geometric description of sublattices*

Let $\Lambda_{\mathbf{A}}$ be a period lattice in $\mathbb{R}^n$ with matrix **A**, and let $\Lambda_{\mathbf{A}}^*$ be the lattice reciprocal to $\Lambda_{\mathbf{A}}$, with period matrix $(A^{-1})^T$. Let $\Lambda_{\mathbf{B}}, \mathbf{B}, \Lambda_{\mathbf{B}}^*$ be defined similarly, and let us suppose that $\Lambda_{\mathbf{A}}$ *is a sublattice of* $\Lambda_{\mathbf{B}}$, *i.e.* that $\Lambda_{\mathbf{B}} \supset \Lambda_{\mathbf{A}}$ as a set.

The relation between $\Lambda_{\mathbf{A}}$ and $\Lambda_{\mathbf{B}}$ may be described in two different fashions: (i) multiplicatively, and (ii) additively.

(i) We may write $\mathbf{A} = \mathbf{BN}$ for some non-singular matrix **N** with integer entries. **N** may be viewed as the period matrix of the coarser lattice $\Lambda_{\mathbf{A}}$ with respect to the period basis of the finer lattice $\Lambda_{\mathbf{B}}$. It will be more convenient to write $\mathbf{A} = \mathbf{DB}$, where $\mathbf{D} = \mathbf{BNB}^{-1}$ is a rational matrix (with integer determinant since $\det \mathbf{D} = \det \mathbf{N}$) in terms of which the two lattices are related by

$$\Lambda_{\mathbf{A}} = \mathbf{D}\Lambda_{\mathbf{B}}.$$

(ii) Call two vectors in $\Lambda_{\mathbf{B}}$ *congruent modulo* $\Lambda_{\mathbf{A}}$ if their difference lies in $\Lambda_{\mathbf{A}}$. Denote the set of congruence classes (or 'cosets') by $\Lambda_{\mathbf{B}}/\Lambda_{\mathbf{A}}$, and the number of these classes by $[\Lambda_{\mathbf{B}} : \Lambda_{\mathbf{A}}]$. The 'coset decomposition'

$$\Lambda_{\mathbf{B}} = \bigcup_{\ell \in \Lambda_{\mathbf{B}}/\Lambda_{\mathbf{A}}} (\ell + \Lambda_{\mathbf{A}})$$

represents $\Lambda_{\mathbf{B}}$ as the disjoint union of $[\Lambda_{\mathbf{B}} : \Lambda_{\mathbf{A}}]$ translates of $\Lambda_{\mathbf{A}}$. $\Lambda_{\mathbf{B}}/\Lambda_{\mathbf{A}}$ is a finite lattice with $[\Lambda_{\mathbf{B}} : \Lambda_{\mathbf{A}}]$ elements, called the *residual lattice* of $\Lambda_{\mathbf{B}}$ modulo $\Lambda_{\mathbf{A}}$.

The two descriptions are connected by the relation $[\Lambda_{\mathbf{B}} : \Lambda_{\mathbf{A}}] = \det \mathbf{D} = \det \mathbf{N}$, which follows from a volume calculation. We may also combine (i) and (ii) into

$$\text{(iii)} \qquad \Lambda_{\mathbf{B}} = \bigcup_{\ell \in \Lambda_{\mathbf{B}}/\Lambda_{\mathbf{A}}} (\ell + \mathbf{D}\Lambda_{\mathbf{B}})$$

which may be viewed as the n-dimensional equivalent of the Euclidean algorithm for integer division: ℓ is the 'remainder' of the division by $\Lambda_{\mathbf{A}}$ of a vector in $\Lambda_{\mathbf{B}}$, the quotient being the matrix **D**.

1.3.2.7.2.2. *Sublattice relations for reciprocal lattices*

Let us now consider the two *reciprocal lattices* $\Lambda_{\mathbf{A}}^*$ and $\Lambda_{\mathbf{B}}^*$. Their period matrices $(\mathbf{A}^{-1})^T$ and $(\mathbf{B}^{-1})^T$ are related by: $(\mathbf{B}^{-1})^T = (\mathbf{A}^{-1})^T\mathbf{N}^T$, where $\mathbf{N}^T$ is an integer matrix; or equivalently by $(\mathbf{B}^{-1})^T = \mathbf{D}^T(\mathbf{A}^{-1})^T$. This shows that the roles are reversed in that $\Lambda_{\mathbf{B}}^*$ *is a sublattice of* $\Lambda_{\mathbf{A}}^*$, which we may write:

$$\text{(i)}^* \qquad \Lambda_{\mathbf{B}}^* = \mathbf{D}^T\Lambda_{\mathbf{A}}^*$$

$$\text{(ii)}^* \qquad \Lambda_{\mathbf{A}}^* = \bigcup_{\ell^* \in \Lambda_{\mathbf{A}}^*/\Lambda_{\mathbf{B}}^*} (\ell^* + \Lambda_{\mathbf{B}}^*).$$

The residual lattice $\Lambda_{\mathbf{A}}^*/\Lambda_{\mathbf{B}}^*$ is finite, with $[\Lambda_{\mathbf{A}}^* : \Lambda_{\mathbf{B}}^*] = \det \mathbf{D} = \det \mathbf{N} = [\Lambda_{\mathbf{B}} : \Lambda_{\mathbf{A}}]$, and we may again combine (i)* and (ii)* into

$$\text{(iii)}^* \qquad \Lambda_{\mathbf{A}}^* = \bigcup_{\ell^* \in \Lambda_{\mathbf{A}}^*/\Lambda_{\mathbf{B}}^*} (\ell^* + \mathbf{D}^T\Lambda_{\mathbf{A}}^*).$$

1.3.2.7.2.3. *Relation between lattice distributions*

The above relations between lattices may be rewritten in terms of the corresponding *lattice distributions* as follows:

$$\text{(i)} \qquad R_{\mathbf{A}} = \frac{1}{|\det \mathbf{D}|}\mathbf{D}^{\#}R_{\mathbf{B}}^*$$

$$\text{(ii)} \qquad R_{\mathbf{B}} = T_{\mathbf{B}/\mathbf{A}} * R_{\mathbf{A}}$$

$$\text{(i)}^* \qquad R_{\mathbf{B}}^* = \frac{1}{|\det \mathbf{D}|}(\mathbf{D}^T)^{\#}R_{\mathbf{A}}^*$$

$$\text{(ii)}^* \qquad R_{\mathbf{A}}^* = T_{\mathbf{A}/\mathbf{B}}^* * R_{\mathbf{B}}^*$$

where

$$T_{\mathbf{B}/\mathbf{A}} = \sum_{\ell \in \Lambda_{\mathbf{B}}/\Lambda_{\mathbf{A}}} \delta_{(\ell)}$$

and

$$T_{\mathbf{A}/\mathbf{B}}^* = \sum_{\ell^* \in \Lambda_{\mathbf{A}}^*/\Lambda_{\mathbf{B}}^*} \delta_{(\ell^*)}$$

are (finite) residual-lattice distributions. We may incorporate the factor $1/|\det \mathbf{D}|$ in (i) and (i)* into these distributions and define

$$S_{\mathbf{B}/\mathbf{A}} = \frac{1}{|\det \mathbf{D}|}T_{\mathbf{B}/\mathbf{A}}, \quad S_{\mathbf{A}/\mathbf{B}}^* = \frac{1}{|\det \mathbf{D}|}T_{\mathbf{A}/\mathbf{B}}^*.$$

Since $|\det \mathbf{D}| = [\Lambda_{\mathbf{B}} : \Lambda_{\mathbf{A}}] = [\Lambda_{\mathbf{A}}^* : \Lambda_{\mathbf{B}}^*]$, convolution with $S_{\mathbf{B}/\mathbf{A}}$ and $S_{\mathbf{A}/\mathbf{B}}^*$ has the effect of *averaging* the translates of a distribution under the elements (or 'cosets') of the residual lattices $\Lambda_{\mathbf{B}}/\Lambda_{\mathbf{A}}$ and $\Lambda_{\mathbf{A}}^*/\Lambda_{\mathbf{B}}^*$, respectively. This process will be called 'coset averaging'. Eliminating $R_{\mathbf{A}}$ and $R_{\mathbf{B}}$ between (i) and (ii), and $R_{\mathbf{A}}^*$ and $R_{\mathbf{B}}^*$ between (i)* and (ii)*, we may write:

$$\text{(i}'\text{)} \qquad R_{\mathbf{A}} = \mathbf{D}^{\#}(S_{\mathbf{B}/\mathbf{A}} * R_{\mathbf{A}})$$

$$\text{(ii}'\text{)} \qquad R_{\mathbf{B}} = S_{\mathbf{B}/\mathbf{A}} * (\mathbf{D}^{\#}R_{\mathbf{B}})$$

$$\text{(i}'\text{)}^* \qquad R_{\mathbf{B}}^* = (\mathbf{D}^T)^{\#}(S_{\mathbf{A}/\mathbf{B}}^* * R_{\mathbf{B}}^*)$$

$$\text{(ii}'\text{)}^* \qquad R_{\mathbf{A}}^* = S_{\mathbf{A}/\mathbf{B}}^* * [(\mathbf{D}^T)^{\#}R_{\mathbf{A}}^*].$$

These identities show that *period subdivision* by convolution with

references