International Tables for Crystallography (2006). Vol. B, Section 1.3.2.7.2.3, pp. 46–47.

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 $\Lambda_{\mathbf{B}}$, **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:

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

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

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

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

These identities show that *period subdivision* by convolution with

$S_{\mathbf{B}/\mathbf{A}}$ (respectively $S^*_{\mathbf{A}/\mathbf{B}}$) on the one hand, and *period decimation* by 'dilation' by $\mathbf{D}^\#$ on the other hand, are mutually inverse operations on $R_\mathbf{A}$ and $R_\mathbf{B}$ (respectively $R^*_\mathbf{A}$ and $R^*_\mathbf{B}$).

1.3.2.7.2.4. *Relation between Fourier transforms*

Finally, let us consider the relations between the *Fourier transforms* of these lattice distributions. Recalling the basic relation of Section 1.3.2.6.5,

$$\begin{aligned}\mathscr{F}[R_\mathbf{A}] &= \frac{1}{|\det \mathbf{A}|} R^*_\mathbf{A} \\ &= \frac{1}{|\det \mathbf{DB}|} T^*_{\mathbf{A}/\mathbf{B}} * R^*_\mathbf{B} \qquad \text{by (ii)}^* \\ &= \left(\frac{1}{|\det \mathbf{D}|} T^*_{\mathbf{A}/\mathbf{B}}\right) * \left(\frac{1}{|\det \mathbf{B}|} R^*_\mathbf{B}\right)\end{aligned}$$

i.e.

(iv) $$\mathscr{F}[R_\mathbf{A}] = S^*_{\mathbf{A}/\mathbf{B}} * \mathscr{F}[R_\mathbf{B}]$$

and similarly:

(v) $$\mathscr{F}[R^*_\mathbf{B}] = S_{\mathbf{B}/\mathbf{A}} * \mathscr{F}[R^*_\mathbf{A}].$$

Thus $R_\mathbf{A}$ (respectively $R^*_\mathbf{B}$), a *decimated* version of $R_\mathbf{B}$ (respectively $R^*_\mathbf{A}$), is transformed by $\mathscr{F}$ into a *subdivided* version of $\mathscr{F}[R_\mathbf{B}]$ (respectively $\mathscr{F}[R^*_\mathbf{A}]$).

The converse is also true:

$$\begin{aligned}\mathscr{F}[R_\mathbf{B}] &= \frac{1}{|\det \mathbf{B}|} R^*_\mathbf{B} \\ &= \frac{1}{|\det \mathbf{B}|}\frac{1}{|\det \mathbf{D}|} (\mathbf{D}^T)^\# R^*_\mathbf{A} \qquad \text{by (i)}^* \\ &= (\mathbf{D}^T)^\# \left(\frac{1}{|\det \mathbf{A}|} R^*_\mathbf{A}\right)\end{aligned}$$

i.e.

(iv′) $$\mathscr{F}[R_\mathbf{B}] = (\mathbf{D}^T)^\# \mathscr{F}[R_\mathbf{A}]$$

and similarly

(v′) $$\mathscr{F}[R^*_\mathbf{A}] = \mathbf{D}^\# \mathscr{F}[R^*_\mathbf{B}].$$

Thus $R_\mathbf{B}$ (respectively $R^*_\mathbf{A}$), a *subdivided* version of $R_\mathbf{A}$ (respectively $R^*_\mathbf{B}$) is transformed by $\mathscr{F}$ into a *decimated* version of $\mathscr{F}[R_\mathbf{A}]$ (respectively $\mathscr{F}[R^*_\mathbf{B}]$). Therefore, *the Fourier transform exchanges subdivision and decimation of period lattices for lattice distributions*.

Further insight into this phenomenon is provided by applying $\bar{\mathscr{F}}$ to both sides of (iv) and (v) and invoking the convolution theorem:

(iv″) $$R_\mathbf{A} = \bar{\mathscr{F}}[S^*_{\mathbf{A}/\mathbf{B}}] \times R_\mathbf{B}$$

(v″) $$R^*_\mathbf{B} = \bar{\mathscr{F}}[S_{\mathbf{B}/\mathbf{A}}] \times R^*_\mathbf{A}.$$

These identities show that multiplication by the transform of the period-subdividing distribution $S^*_{\mathbf{A}/\mathbf{B}}$ (respectively $S_{\mathbf{B}/\mathbf{A}}$) has the effect of decimating $R_\mathbf{B}$ to $R_\mathbf{A}$ (respectively $R^*_\mathbf{A}$ to $R^*_\mathbf{B}$). They clearly imply that, if $\ell \in \Lambda_\mathbf{B}/\Lambda_\mathbf{A}$ and $\ell^* \in \Lambda^*_\mathbf{A}/\Lambda^*_\mathbf{B}$, then

$$\begin{aligned}\bar{\mathscr{F}}[S^*_{\mathbf{A}/\mathbf{B}}](\ell) &= 1 \text{ if } \ell = \mathbf{0} \quad (\textit{i.e.}\text{ if } \ell \text{ belongs to the class of } \Lambda_\mathbf{A}), \\ &= 0 \text{ if } \ell \neq \mathbf{0}; \\ \bar{\mathscr{F}}[S_{\mathbf{B}/\mathbf{A}}](\ell^*) &= 1 \text{ if } \ell^* = \mathbf{0} \quad (\textit{i.e.}\text{ if } \ell^* \text{ belongs to the class of } \Lambda^*_\mathbf{B}), \\ &= 0 \text{ if } \ell^* \neq \mathbf{0}.\end{aligned}$$

Therefore, the duality between subdivision and decimation may be viewed as another aspect of that between convolution and multiplication.

There is clearly a strong analogy between the sampling/periodization duality of Section 1.3.2.6.6 and the decimation/subdivision duality, which is viewed most naturally in terms of subgroup relationships: both sampling and decimation involve restricting a function to a *discrete additive subgroup* of the domain over which it is initially given.

1.3.2.7.2.5. *Sublattice relations in terms of periodic distributions*

The usual presentation of this duality is not in terms of lattice distributions, but of periodic distributions obtained by convolving them with a motif.

Given $T^0 \in \mathscr{E}'(\mathbb{R}^n)$, let us form $R_\mathbf{A} * T^0$, then *decimate* its transform $(1/|\det \mathbf{A}|)R^*_\mathbf{A} \times \bar{\mathscr{F}}[T^0]$ by keeping only its values at the points of the coarser lattice $\Lambda^*_\mathbf{B} = \mathbf{D}^T\Lambda^*_\mathbf{A}$; as a result, $R^*_\mathbf{A}$ is replaced by $(1/|\det \mathbf{D}|)R^*_\mathbf{B}$, and the reverse transform then yields

$$\frac{1}{|\det \mathbf{D}|} R_\mathbf{B} * T^0 = S_{\mathbf{B}/\mathbf{A}} * (R_\mathbf{A} * T^0) \qquad \text{by (ii)},$$

which is the *coset-averaged* version of the original $R_\mathbf{A} * T^0$. The converse situation is analogous to that of Shannon's sampling theorem. Let a function $\varphi \in \mathscr{E}(\mathbb{R}^n)$ whose transform $\Phi = \mathscr{F}[\varphi]$ has compact support be sampled as $R_\mathbf{B} \times \varphi$ at the nodes of $\Lambda_\mathbf{B}$. Then

$$\mathscr{F}[R_\mathbf{B} \times \varphi] = \frac{1}{|\det \mathbf{B}|}(R^*_\mathbf{B} * \Phi)$$

is periodic with period lattice $\Lambda^*_\mathbf{B}$. If the sampling lattice $\Lambda_\mathbf{B}$ is decimated to $\Lambda_\mathbf{A} = \mathbf{D}\Lambda_\mathbf{B}$, the inverse transform becomes

$$\begin{aligned}\mathscr{F}[R_\mathbf{A} \times \varphi] &= \frac{1}{|\det \mathbf{D}|}(R^*_\mathbf{A} * \Phi) \\ &= S^*_{\mathbf{A}/\mathbf{B}} * (R^*_\mathbf{B} * \Phi) \qquad \text{by (ii)}^*,\end{aligned}$$

hence becomes periodized more finely by averaging over the cosets of $\Lambda^*_\mathbf{A}/\Lambda^*_\mathbf{B}$. With this finer periodization, the various copies of Supp Φ may start to overlap (a phenomenon called 'aliasing'), indicating that decimation has produced too coarse a sampling of φ.

1.3.2.7.3. *Discretization of the Fourier transformation*

Let $\varphi^0 \in \mathscr{E}(\mathbb{R}^n)$ be such that $\Phi^0 = \mathscr{F}[\varphi^0]$ has compact support (φ^0 is said to be *band-limited*). Then $\varphi = R_\mathbf{A} * \varphi^0$ is $\Lambda_\mathbf{A}$-periodic, and $\Phi = \mathscr{F}[\varphi] = (1/|\det \mathbf{A}|)R^*_\mathbf{A} \times \Phi^0$ is such that only a finite number of points $\lambda^*_\mathbf{A}$ of $\Lambda^*_\mathbf{A}$ have a non-zero Fourier coefficient $\Phi^0(\lambda^*_\mathbf{A})$ attached to them. We may therefore find a *decimation* $\Lambda^*_\mathbf{B} = \mathbf{D}^T\Lambda^*_\mathbf{A}$ of $\Lambda^*_\mathbf{A}$ such that the distinct translates of Supp Φ^0 by vectors of $\Lambda^*_\mathbf{B}$ do not intersect.

The distribution Φ can be uniquely recovered from $R^*_\mathbf{B} * \Phi$ by the procedure of Section 1.3.2.7.1, and we may write:

$$\begin{aligned}R^*_\mathbf{B} * \Phi &= \frac{1}{|\det \mathbf{A}|} R^*_\mathbf{B} * (R^*_\mathbf{A} \times \Phi^0) \\ &= \frac{1}{|\det \mathbf{A}|} R^*_\mathbf{A} \times (R^*_\mathbf{B} * \Phi^0) \\ &= \frac{1}{|\det \mathbf{A}|} R^*_\mathbf{B} * [T^*_{\mathbf{A}/\mathbf{B}} \times (R^*_\mathbf{B} * \Phi^0)];\end{aligned}$$

these rearrangements being legitimate because Φ^0 and $T^*_{\mathbf{A}/\mathbf{B}}$ have compact supports which are intersection-free under the action of $\Lambda^*_\mathbf{B}$. By virtue of its $\Lambda^*_\mathbf{B}$-periodicity, this distribution is entirely characterized by its 'motif' $\tilde{\Phi}$ with respect to $\Lambda^*_\mathbf{B}$:

references