International Tables for Crystallography (2006). Vol. B, Section 1.3.2.7.3, pp. 47–48.

$S_{\mathbf{B}/\mathbf{A}}$ (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.

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

and similarly:

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

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.

$$\text{(iv}'\text{)} \qquad \mathscr{F}[R_{\mathbf{B}}] = (\mathbf{D}^T)^{\#}\mathscr{F}[R_{\mathbf{A}}]$$

and similarly

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

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:

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

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

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

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

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 $\Lambda^*_{\mathbf{B}}$:

$$\tilde{\Phi} = \frac{1}{|\det \mathbf{A}|} T^*_{\mathbf{A}/\mathbf{B}} \times (R^*_{\mathbf{B}} * \Phi^0).$$

Similarly, φ may be uniquely recovered by Shannon interpolation from the distribution sampling its values at the nodes of $\Lambda_{\mathbf{B}} = \mathbf{D}^{-1}\Lambda_{\mathbf{A}}$ ($\Lambda_{\mathbf{B}}$ is a *subdivision* of $\Lambda_{\mathbf{B}}$). By virtue of its $\Lambda_{\mathbf{A}}$-periodicity, this distribution is completely characterized by its motif:

$$\tilde{\varphi} = T_{\mathbf{B}/\mathbf{A}} \times \varphi = T_{\mathbf{B}/\mathbf{A}} \times (R^*_{\mathbf{A}} * \varphi^0).$$

Let $\boldsymbol{\ell} \in \Lambda_{\mathbf{B}}/\Lambda_{\mathbf{A}}$ and $\boldsymbol{\ell}^* \in \Lambda^*_{\mathbf{A}}/\Lambda^*_{\mathbf{B}}$, and define the two sets of coefficients

(1) $\tilde{\varphi}(\boldsymbol{\ell}) = \varphi(\boldsymbol{\ell} + \boldsymbol{\lambda}_{\mathbf{A}})$ for any $\boldsymbol{\lambda}_{\mathbf{A}} \in \Lambda_{\mathbf{A}}$ (all choices of $\boldsymbol{\lambda}_{\mathbf{A}}$ give the same $\tilde{\varphi}$),

(2) $\tilde{\Phi}(\boldsymbol{\ell}^*) = \Phi^0(\boldsymbol{\ell}^* + \boldsymbol{\lambda}^*_{\mathbf{B}})$ for the unique $\boldsymbol{\lambda}^*_{\mathbf{B}}$ (if it exists) such that $\boldsymbol{\ell}^* + \boldsymbol{\lambda}^*_{\mathbf{B}} \in \operatorname{Supp} \Phi^0$,
$= 0$ if no such $\boldsymbol{\lambda}^*_{\mathbf{B}}$ exists.

Define the two distributions

$$\omega = \sum_{\boldsymbol{\ell} \in \Lambda_{\mathbf{B}}/\Lambda_{\mathbf{A}}} \tilde{\varphi}(\boldsymbol{\ell}) \delta_{(\boldsymbol{\ell})}$$

and

$$\Omega = \sum_{\boldsymbol{\ell}^* \in \Lambda^*_{\mathbf{A}}/\Lambda^*_{\mathbf{B}}} \tilde{\Phi}(\boldsymbol{\ell}^*) \delta_{(\boldsymbol{\ell}^*)}.$$

The relation between ω and Ω has two equivalent forms:

(i) $$R_{\mathbf{A}} * \omega = \mathscr{F}[R^*_{\mathbf{B}} * \Omega]$$

(ii) $$\bar{\mathscr{F}}[R_{\mathbf{A}} * \omega] = R^*_{\mathbf{B}} * \Omega.$$

By (i), $R_{\mathbf{A}} * \omega = |\det \mathbf{B}| R_{\mathbf{B}} \times \mathscr{F}[\Omega]$. Both sides are weighted lattice distributions concentrated at the nodes of $\Lambda_{\mathbf{B}}$, and equating the weights at $\boldsymbol{\lambda}_{\mathbf{B}} = \boldsymbol{\ell} + \boldsymbol{\lambda}_{\mathbf{A}}$ gives

$$\tilde{\varphi}(\boldsymbol{\ell}) = \frac{1}{|\det \mathbf{D}|} \sum_{\boldsymbol{\ell}^* \in \Lambda^*_{\mathbf{A}}/\Lambda^*_{\mathbf{B}}} \tilde{\Phi}(\boldsymbol{\ell}^*) \exp[-2\pi i \boldsymbol{\ell}^* \cdot (\boldsymbol{\ell} + \boldsymbol{\lambda}_{\mathbf{A}})].$$

Since $\boldsymbol{\ell}^* \in \Lambda^*_{\mathbf{A}}$, $\boldsymbol{\ell}^* \cdot \boldsymbol{\lambda}_{\mathbf{A}}$ is an integer, hence

$$\tilde{\varphi}(\boldsymbol{\ell}) = \frac{1}{|\det \mathbf{D}|} \sum_{\boldsymbol{\ell}^* \in \Lambda^*_{\mathbf{A}}/\Lambda^*_{\mathbf{B}}} \tilde{\Phi}(\boldsymbol{\ell}^*) \exp(-2\pi i \boldsymbol{\ell}^* \cdot \boldsymbol{\ell}).$$

By (ii), we have

$$\frac{1}{|\det \mathbf{A}|} R^*_{\mathbf{B}} * [T^*_{\mathbf{A}/\mathbf{B}} \times (R^*_{\mathbf{B}} * \Phi^0)] = \frac{1}{|\det \mathbf{A}|} \bar{\mathscr{F}}[R_{\mathbf{A}} * \omega].$$

Both sides are weighted lattice distributions concentrated at the nodes of $\Lambda^*_{\mathbf{B}}$, and equating the weights at $\boldsymbol{\lambda}^*_{\mathbf{A}} = \boldsymbol{\ell}^* + \boldsymbol{\lambda}^*_{\mathbf{B}}$ gives

$$\tilde{\Phi}(\boldsymbol{\ell}^*) = \sum_{\boldsymbol{\ell} \in \Lambda_{\mathbf{B}}/\Lambda_{\mathbf{A}}} \tilde{\varphi}(\boldsymbol{\ell}) \exp[+2\pi i \boldsymbol{\ell} \cdot (\boldsymbol{\ell}^* + \boldsymbol{\lambda}^*_{\mathbf{B}})].$$

Since $\boldsymbol{\ell} \in \Lambda_{\mathbf{B}}$, $\boldsymbol{\ell} \cdot \boldsymbol{\lambda}^*_{\mathbf{B}}$ is an integer, hence

$$\tilde{\Phi}(\boldsymbol{\ell}^*) = \sum_{\boldsymbol{\ell} \in \Lambda_{\mathbf{B}}/\Lambda_{\mathbf{A}}} \tilde{\varphi}(\boldsymbol{\ell}) \exp(+2\pi i \boldsymbol{\ell} \cdot \boldsymbol{\ell}^*).$$

Now the decimation/subdivision relations between $\Lambda_{\mathbf{A}}$ and $\Lambda_{\mathbf{B}}$ may be written:

$$\mathbf{A} = \mathbf{DB} = \mathbf{BN},$$

so that

$$\boldsymbol{\ell} = \mathbf{B}\boldsymbol{k} \qquad \text{for } \boldsymbol{k} \in \mathbb{Z}^n$$

$$\boldsymbol{\ell}^* = (\mathbf{A}^{-1})^T \boldsymbol{k}^* \qquad \text{for } \boldsymbol{k}^* \in \mathbb{Z}^n$$

with $(\mathbf{A}^{-1})^T = (\mathbf{B}^{-1})^T (\mathbf{N}^{-1})^T$, hence finally

$$\boldsymbol{\ell}^* \cdot \boldsymbol{\ell} = \boldsymbol{\ell} \cdot \boldsymbol{\ell}^* = \boldsymbol{k}^* \cdot (\mathbf{N}^{-1}\boldsymbol{k}).$$

Denoting $\tilde{\varphi}(\mathbf{B}\boldsymbol{k})$ by $\psi(\boldsymbol{k})$ and $\tilde{\Phi}[(\mathbf{A}^{-1})^T \boldsymbol{k}^*]$ by $\Psi(\boldsymbol{k}^*)$, the relation between ω and Ω may be written in the equivalent form

(i) $$\psi(\boldsymbol{k}) = \frac{1}{|\det \mathbf{N}|} \sum_{\boldsymbol{k}^* \in \mathbb{Z}^n/\mathbf{N}^T\mathbb{Z}^n} \Psi(\boldsymbol{k}^*) \exp[-2\pi i \boldsymbol{k}^* \cdot (\mathbf{N}^{-1}\boldsymbol{k})]$$

(ii) $$\Psi(\boldsymbol{k}^*) = \sum_{\boldsymbol{k} \in \mathbb{Z}^n/\mathbf{N}\mathbb{Z}^n} \psi(\boldsymbol{k}) \exp[+2\pi i \boldsymbol{k}^* \cdot (\mathbf{N}^{-1}\boldsymbol{k})],$$

where the summations are now over *finite* residual lattices in standard form.

Equations (i) and (ii) describe two mutually inverse linear transformations $\mathscr{F}(\mathbf{N})$ and $\bar{\mathscr{F}}(\mathbf{N})$ between two vector spaces $W_{\mathbf{N}}$ and $W^*_{\mathbf{N}}$ of dimension $|\det \mathbf{N}|$. $\mathscr{F}(\mathbf{N})$ [respectively $\bar{\mathscr{F}}(\mathbf{N})$] is the *discrete* Fourier (respectively inverse Fourier) transform associated to matrix $\mathbf{N}$.

The vector spaces $W_{\mathbf{N}}$ and $W^*_{\mathbf{N}}$ may be viewed from two different standpoints:

(1) as vector spaces of *weighted residual-lattice distributions*, of the form $\alpha(\mathbf{x})T_{\mathbf{B}/\mathbf{A}}$ and $\beta(\mathbf{x})T^*_{\mathbf{A}/\mathbf{B}}$; the canonical basis of $W_{\mathbf{N}}$ (respectively $W^*_{\mathbf{N}}$) then consists of the $\delta_{(\boldsymbol{k})}$ for $\boldsymbol{k} \in \mathbb{Z}^n/\mathbf{N}\mathbb{Z}^n$ [respectively $\delta_{(\boldsymbol{k}^*)}$ for $\boldsymbol{k}^* \in \mathbb{Z}^n/\mathbf{N}^T\mathbb{Z}^n$];

(2) as vector spaces of *weight vectors* for the $|\det \mathbf{N}|$ δ-functions involved in the expression for $T_{\mathbf{B}/\mathbf{A}}$ (respectively $T^*_{\mathbf{A}/\mathbf{B}}$); the canonical basis of $W_{\mathbf{N}}$ (respectively $W^*_{\mathbf{N}}$) consists of weight vectors $\mathbf{u}_{\boldsymbol{k}}$ (respectively $\mathbf{v}_{\boldsymbol{k}^*}$) giving weight 1 to element $\boldsymbol{k}$ (respectively $\boldsymbol{k}^*$) and 0 to the others.

These two spaces are said to be 'isomorphic' (a relation denoted $\cong$), the isomorphism being given by the one-to-one correspondence:

$$\omega = \sum_{\boldsymbol{k}} \psi(\boldsymbol{k}) \delta_{(\boldsymbol{k})} \quad \leftrightarrow \quad \psi = \sum_{\boldsymbol{k}} \psi(\boldsymbol{k}) \mathbf{u}_{\boldsymbol{k}}$$

$$\Omega = \sum_{\boldsymbol{k}^*} \Psi(\boldsymbol{k}^*) \delta_{(\boldsymbol{k}^*)} \quad \leftrightarrow \quad \Psi = \sum_{\boldsymbol{k}^*} \Psi(\boldsymbol{k}^*) \mathbf{v}_{\boldsymbol{k}^*}.$$

The second viewpoint will be adopted, as it involves only linear algebra. However, it is most helpful to keep the first one in mind and to think of the data or results of a discrete Fourier transform as representing (through their sets of unique weights) two periodic lattice distributions related by the full, distribution-theoretic Fourier transform.

We therefore view $W_{\mathbf{N}}$ (respectively $W^*_{\mathbf{N}}$) as the vector space of complex-valued functions over the finite residual lattice $\Lambda_{\mathbf{B}}/\Lambda_{\mathbf{A}}$ (respectively $\Lambda^*_{\mathbf{A}}/\Lambda^*_{\mathbf{B}}$) and write:

$$W_{\mathbf{N}} \cong L(\Lambda_{\mathbf{B}}/\Lambda_{\mathbf{A}}) \cong L(\mathbb{Z}^n/\mathbf{N}\mathbb{Z}^n)$$

$$W^*_{\mathbf{N}} \cong L(\Lambda^*_{\mathbf{A}}/\Lambda^*_{\mathbf{B}}) \cong L(\mathbb{Z}^n/\mathbf{N}^T\mathbb{Z}^n)$$

since a vector such as ψ is in fact the function $\boldsymbol{k} \longmapsto \psi(\boldsymbol{k})$.

The two spaces $W_{\mathbf{N}}$ and $W^*_{\mathbf{N}}$ may be equipped with the following Hermitian inner products:

$$(\varphi, \psi)_W = \sum_{\boldsymbol{k}} \overline{\varphi(\boldsymbol{k})} \psi(\boldsymbol{k})$$

$$(\Phi, \Psi)_{W^*} = \sum_{\boldsymbol{k}} \overline{\Phi(\boldsymbol{k}^*)} \Psi(\boldsymbol{k}^*),$$

which makes each of them into a *Hilbert space*. The canonical bases $\{\mathbf{u}_{\boldsymbol{k}} | \boldsymbol{k} \in \mathbb{Z}^n/\mathbf{N}\mathbb{Z}^n\}$ and $\{\mathbf{v}_{\boldsymbol{k}^*} | \boldsymbol{k}^* \in \mathbb{Z}^n/\mathbf{N}^T\mathbb{Z}^n\}$ and $W_{\mathbf{N}}$ and $W^*_{\mathbf{N}}$ are *orthonormal* for their respective product.

references