

1.3. FOURIER TRANSFORMS IN CRYSTALLOGRAPHY

$S_{B/A}$ (respectively $S_{A/B}^*$) on the one hand, and *period decimation* by ‘dilation’ by $\mathbf{D}^\#$ on the other hand, are mutually inverse operations on R_A and R_B (respectively R_A^* and R_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,

$$\begin{aligned}\mathcal{F}[R_A] &= \frac{1}{|\det \mathbf{A}|} R_A^* \\ &= \frac{1}{|\det \mathbf{DB}|} T_{A/B}^* * R_B^* \quad \text{by (ii)*} \\ &= \left(\frac{1}{|\det \mathbf{D}|} T_{A/B}^* \right) * \left(\frac{1}{|\det \mathbf{B}|} R_B^* \right)\end{aligned}$$

i.e.

$$(iv) \quad \mathcal{F}[R_A] = S_{A/B}^* * \mathcal{F}[R_B]$$

and similarly:

$$(v) \quad \mathcal{F}[R_B] = S_{B/A} * \mathcal{F}[R_A^*].$$

Thus R_A (respectively R_B^*), a *decimated* version of R_B (respectively R_A^*), is transformed by \mathcal{F} into a *subdivided* version of $\mathcal{F}[R_B]$ (respectively $\mathcal{F}[R_A^*]$).

The converse is also true:

$$\begin{aligned}\mathcal{F}[R_B] &= \frac{1}{|\det \mathbf{B}|} R_B^* \\ &= \frac{1}{|\det \mathbf{B}|} \frac{1}{|\det \mathbf{D}|} (\mathbf{D}^T)^\# R_A^* \quad \text{by (i)*} \\ &= (\mathbf{D}^T)^\# \left(\frac{1}{|\det \mathbf{A}|} R_A^* \right)\end{aligned}$$

i.e.

$$(iv') \quad \mathcal{F}[R_B] = (\mathbf{D}^T)^\# \mathcal{F}[R_A]$$

and similarly

$$(v') \quad \mathcal{F}[R_A^*] = \mathbf{D}^\# \mathcal{F}[R_B^*].$$

Thus R_B (respectively R_A^*), a *subdivided* version of R_A (respectively R_B^*) is transformed by \mathcal{F} into a *decimated* version of $\mathcal{F}[R_A]$ (respectively $\mathcal{F}[R_B^*]$). Therefore, *the Fourier transform exchanges subdivision and decimation of period lattices for lattice distributions.*

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

$$(iv'') \quad R_A = \tilde{\mathcal{F}}[S_{A/B}^*] \times R_B$$

$$(v'') \quad R_B^* = \tilde{\mathcal{F}}[S_{B/A}] \times R_A^*.$$

These identities show that multiplication by the transform of the period-subdividing distribution $S_{A/B}^*$ (respectively $S_{B/A}$) has the effect of decimating R_B to R_A (respectively R_A^* to R_B^*). They clearly imply that, if $\ell \in \Lambda_B/\Lambda_A$ and $\ell^* \in \Lambda_A^*/\Lambda_B^*$, then

$$\begin{aligned}\tilde{\mathcal{F}}[S_{A/B}^*](\ell) &= 1 \text{ if } \ell = \mathbf{0} \quad (\text{i.e. if } \ell \text{ belongs} \\ &\quad \text{to the class of } \Lambda_A), \\ &= 0 \text{ if } \ell \neq \mathbf{0};\end{aligned}$$

$$\begin{aligned}\tilde{\mathcal{F}}[S_{B/A}](\ell^*) &= 1 \text{ if } \ell^* = \mathbf{0} \quad (\text{i.e. if } \ell^* \text{ belongs} \\ &\quad \text{to the class of } \Lambda_B^*), \\ &= 0 \text{ if } \ell^* \neq \mathbf{0}.\end{aligned}$$

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

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

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

$$\mathcal{F}[R_B \times \varphi] = \frac{1}{|\det \mathbf{B}|} (R_B^* * \Phi)$$

is periodic with period lattice Λ_B^* . If the sampling lattice Λ_B is decimated to $\Lambda_A = \mathbf{D}\Lambda_B$, the inverse transform becomes

$$\begin{aligned}\mathcal{F}[R_A \times \varphi] &= \frac{1}{|\det \mathbf{D}|} (R_A^* * \Phi) \\ &= S_{A/B}^* * (R_B^* * \Phi) \quad \text{by (ii)*,}\end{aligned}$$

hence becomes periodized more finely by averaging over the cosets of Λ_A^*/Λ_B^* . With this finer periodization, the various copies of $\text{Supp } \Phi$ 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 $\varphi^0 \in \mathcal{E}(\mathbb{R}^n)$ be such that $\Phi^0 = \tilde{\mathcal{F}}[\varphi^0]$ has compact support (φ^0 is said to be *band-limited*). Then $\varphi = R_A * \varphi^0$ is Λ_A -periodic, and $\Phi = \tilde{\mathcal{F}}[\varphi] = (1/|\det \mathbf{A}|)R_A^* \times \Phi^0$ is such that only a finite number of points λ_A^* of Λ_A^* have a non-zero Fourier coefficient $\Phi^0(\lambda_A^*)$ attached to them. We may therefore find a *decimation* $\Lambda_B^* = \mathbf{D}^T \Lambda_A^*$ of Λ_A^* such that the distinct translates of $\text{Supp } \Phi^0$ by vectors of Λ_B^* do not intersect.

The distribution Φ can be uniquely recovered from $R_B^* * \Phi$ by the procedure of Section 1.3.2.7.1, and we may write:

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

these rearrangements being legitimate because Φ^0 and $T_{A/B}^*$ have compact supports which are intersection-free under the action of Λ_B^* . By virtue of its Λ_B^* -periodicity, this distribution is entirely characterized by its ‘motif’ Φ with respect to Λ_B^* :