

1.3. FOURIER TRANSFORMS IN CRYSTALLOGRAPHY

The Poisson kernel

$$P_r(x) = 1 + 2 \sum_{m=1}^{\infty} r^m \cos 2\pi mx$$

$$= \frac{1 - r^2}{1 - 2r \cos 2\pi mx + r^2}$$

with $0 \leq r < 1$ gives rise to an Abel summation procedure [Tolstov (1962, p. 162); Whittaker & Watson (1927, p. 57)] since

$$(P_r * f)(x) = \sum_{m \in \mathbb{Z}} c_m(f) r^{|m|} \exp(2\pi imx).$$

Compared with the other kernels, P_r has the disadvantage of not being a trigonometric polynomial; however, P_r is the real part of the Cauchy kernel (Cartan, 1961; Ahlfors, 1966):

$$P_r(x) = \Re \left[\frac{1 + r \exp(2\pi ix)}{1 - r \exp(2\pi ix)} \right]$$

and hence provides a link between trigonometric series and analytic functions of a complex variable.

Other methods of summation involve forming a moving average of f by convolution with other sequences of functions $\alpha_p(\mathbf{x})$ besides D_p of F_p which ‘tend towards δ ’ as $p \rightarrow \infty$. The convolution is performed by multiplying the Fourier coefficients of f by those of α_p , so that one forms the quantities

$$S'_p(f)(x) = \sum_{|m| \leq p} c_m(\alpha_p) c_m(f) \exp(2\pi imx).$$

For instance the ‘sigma factors’ of Lanczos (Lanczos, 1966, p. 65), defined by

$$\sigma_m = \frac{\sin[m\pi/p]}{m\pi/p},$$

lead to a summation procedure whose behaviour is intermediate between those using the Dirichlet and the Fejér kernels; it corresponds to forming a moving average of f by convolution with

$$\alpha_p = P\chi_{[-1/(2p), 1/(2p)]} * D_p,$$

which is itself the convolution of a ‘rectangular pulse’ of width $1/p$ and of the Dirichlet kernel of order p .

A review of the summation problem in crystallography is given in Section 1.3.4.2.1.3.

1.3.2.6.10.2. Classical L^2 theory

The space $L^2(\mathbb{R}/\mathbb{Z})$ of (equivalence classes of) square-integrable complex-valued functions f on the circle is contained in $L^1(\mathbb{R}/\mathbb{Z})$, since by the Cauchy–Schwarz inequality

$$\|f\|_1^2 = \left(\int_0^1 |f(x)| \times 1 \, dx \right)^2$$

$$\leq \left(\int_0^1 |f(x)|^2 \, dx \right) \left(\int_0^1 1^2 \, dx \right) = \|f\|_2^2 \leq \infty.$$

Thus all the results derived for L^1 hold for L^2 , a great simplification over the situation in \mathbb{R} or \mathbb{R}^n where neither L^1 nor L^2 was contained in the other.

However, more can be proved in L^2 , because L^2 is a Hilbert space (Section 1.3.2.2.4) for the inner product

$$(f, g) = \int_0^1 \overline{f(x)} g(x) \, dx,$$

and because the family of functions $\{\exp(2\pi imx)\}_{m \in \mathbb{Z}}$ constitutes an orthonormal Hilbert basis for L^2 .

The sequence of Fourier coefficients $c_m(f)$ of $f \in L^2$ belongs to the space $\ell^2(\mathbb{Z})$ of square-summable sequences:

$$\sum_{m \in \mathbb{Z}} |c_m(f)|^2 < \infty.$$

Conversely, every element $c = (c_m)$ of ℓ^2 is the sequence of Fourier coefficients of a unique function in L^2 . The inner product

$$(c, d) = \sum_{m \in \mathbb{Z}} \overline{c_m} d_m$$

makes ℓ^2 into a Hilbert space, and the map from L^2 to ℓ^2 established by the Fourier transformation is an isometry (Parseval/Plancherel):

$$\|f\|_{L^2} = \|c(f)\|_{\ell^2}$$

or equivalently:

$$(f, g) = (c(f), c(g)).$$

This is a useful property in applications, since (f, g) may be calculated either from f and g themselves, or from their Fourier coefficients $c(f)$ and $c(g)$ (see Section 1.3.4.4.6) for crystallographic applications).

By virtue of the orthogonality of the basis $\{\exp(2\pi imx)\}_{m \in \mathbb{Z}}$, the partial sum $S_p(f)$ is the best mean-square fit to f in the linear subspace of L^2 spanned by $\{\exp(2\pi imx)\}_{|m| \leq p}$, and hence (Bessel’s inequality)

$$\sum_{|m| \leq p} |c_m(f)|^2 = \|f\|_2^2 - \sum_{|M| \geq p} |c_M(f)|^2 \leq \|f\|_2^2.$$

1.3.2.6.10.3. The viewpoint of distribution theory

The use of distributions enlarges considerably the range of behaviour which can be accommodated in a Fourier series, even in the case of general dimension n where classical theories meet with even more difficulties than in dimension 1.

Let $\{w_m\}_{m \in \mathbb{Z}}$ be a sequence of complex numbers with $|w_m|$ growing at most polynomially as $|m| \rightarrow \infty$, say $|w_m| \leq C|m|^K$. Then the sequence $\{w_m/(2\pi im)^{K+2}\}_{m \in \mathbb{Z}}$ is in ℓ^2 and even defines a continuous function $f \in L^2(\mathbb{R}/\mathbb{Z})$ and an associated tempered distribution $T_f \in \mathcal{D}'(\mathbb{R}/\mathbb{Z})$. Differentiation of T_f ($K+2$) times then yields a tempered distribution whose Fourier transform leads to the original sequence of coefficients. Conversely, by the structure theorem for distributions with compact support (Section 1.3.2.3.9.7), the motif T^0 of a \mathbb{Z} -periodic distribution is a derivative of finite order of a continuous function; hence its Fourier coefficients will grow at most polynomially with $|m|$ as $|m| \rightarrow \infty$.

Thus distribution theory allows the manipulation of Fourier series whose coefficients exhibit polynomial growth as their order goes to infinity, while those derived from functions had to tend to 0 by virtue of the Riemann–Lebesgue lemma. The distribution-theoretic approach to Fourier series holds even in the case of general dimension n , where classical theories meet with even more difficulties (see Ash, 1976) than in dimension 1.

1.3.2.7. The discrete Fourier transformation

1.3.2.7.1. Shannon’s sampling theorem and interpolation formula

Let $\varphi \in \mathcal{E}(\mathbb{R}^n)$ be such that $\Phi = \mathcal{F}[\varphi]$ has compact support K . Let φ be sampled at the nodes of a lattice Λ^* , yielding the lattice distribution $R^* \times \varphi$. The Fourier transform of this sampled version of φ is

$$\mathcal{F}[R^* \times \varphi] = |\det \mathbf{A}| (R * \Phi),$$

1. GENERAL RELATIONSHIPS AND TECHNIQUES

which is essentially Φ periodized by period lattice $\Lambda = (\Lambda^*)^*$, with period matrix \mathbf{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’ \mathcal{V} of Λ (i.e. a fundamental domain for the action of Λ in \mathbb{R}^n) whose boundary does not meet K . If $\chi_{\mathcal{V}}$ is the indicator function of \mathcal{V} , then

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

Transforming both sides by $\tilde{\mathcal{F}}$ yields

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

i.e.

$$\varphi = \left(\frac{1}{V} \tilde{\mathcal{F}}[\chi_{\mathcal{V}}] \right) * (R * \varphi)$$

since $|\det \mathbf{A}|$ is the volume V of \mathcal{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 $R * \varphi$) 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 \mathbf{A} , and let $\Lambda_{\mathbf{A}}^*$ be the lattice reciprocal to $\Lambda_{\mathbf{A}}$, with period matrix $(\mathbf{A}^{-1})^T$. 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 $\mathbf{A} = \mathbf{B}\mathbf{N}$ for some non-singular matrix \mathbf{N} with integer entries. \mathbf{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 $\mathbf{A} = \mathbf{D}\mathbf{B}$, where $\mathbf{D} = \mathbf{B}\mathbf{N}\mathbf{B}^{-1}$ 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

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

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 \mathbf{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:

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

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

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

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

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:

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

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

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

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

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:

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

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

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

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

These identities show that period subdivision by convolution with

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

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

$$= 0 \text{ if } \ell \neq \mathbf{0};$$

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

$$= 0 \text{ if } \ell^* \neq \mathbf{0}.$$

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^* :

1. GENERAL RELATIONSHIPS AND TECHNIQUES

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

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

$$\begin{aligned} (1) \quad \tilde{\varphi}(\ell) &= \varphi(\ell + \boldsymbol{\lambda}_{\mathbf{A}}) && \text{for any } \boldsymbol{\lambda}_{\mathbf{A}} \in \Lambda_{\mathbf{A}} \\ &&& \text{(all choices of } \boldsymbol{\lambda}_{\mathbf{A}} \text{ give the same } \tilde{\varphi}), \\ (2) \quad \tilde{\Phi}(\ell^*) &= \Phi^0(\ell^* + \boldsymbol{\lambda}_{\mathbf{B}}^*) && \text{for the unique } \boldsymbol{\lambda}_{\mathbf{B}}^* \text{ (if it exists)} \\ &&& \text{such that } \ell^* + \boldsymbol{\lambda}_{\mathbf{B}}^* \in \text{Supp } \Phi^0, \\ &= 0 && \text{if no such } \boldsymbol{\lambda}_{\mathbf{B}}^* \text{ exists.} \end{aligned}$$

Define the two distributions

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

and

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

The relation between ω and Ω has two equivalent forms:

$$\begin{aligned} (i) \quad R_{\mathbf{A}} * \omega &= \mathcal{F}[R_{\mathbf{B}}^* * \Omega] \\ (ii) \quad \tilde{\mathcal{F}}[R_{\mathbf{A}} * \omega] &= R_{\mathbf{B}}^* * \Omega. \end{aligned}$$

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

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

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

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

By (ii), we have

$$\frac{1}{|\det \mathbf{A}|} R_{\mathbf{B}}^* * [T_{\mathbf{A}/\mathbf{B}}^* \times (R_{\mathbf{B}}^* * \Phi^0)] = \frac{1}{|\det \mathbf{A}|} \tilde{\mathcal{F}}[R_{\mathbf{A}} * \omega].$$

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

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

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

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

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

$$\mathbf{A} = \mathbf{D}\mathbf{B} = \mathbf{B}\mathbf{N},$$

so that

$$\begin{aligned} \ell &= \mathbf{B}\boldsymbol{k} && \text{for } \boldsymbol{k} \in \mathbb{Z}^n \\ \ell^* &= (\mathbf{A}^{-1})^T \boldsymbol{k}^* && \text{for } \boldsymbol{k}^* \in \mathbb{Z}^n \end{aligned}$$

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

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

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

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

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

Equations (i) and (ii) describe two mutually inverse linear transformations $\mathcal{F}(\mathbf{N})$ and $\tilde{\mathcal{F}}(\mathbf{N})$ between two vector spaces $W_{\mathbf{N}}$ and $W_{\mathbf{N}}^*$ of dimension $|\det \mathbf{N}|$. $\mathcal{F}(\mathbf{N})$ [respectively $\tilde{\mathcal{F}}(\mathbf{N})$] 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:

$$\begin{aligned} \omega = \sum_{\boldsymbol{k}} \psi(\boldsymbol{k}) \delta_{(\boldsymbol{k})} &\leftrightarrow \psi = \sum_{\boldsymbol{k}} \psi(\boldsymbol{k}) \mathbf{u}_{\boldsymbol{k}} \\ \Omega = \sum_{\boldsymbol{k}^*} \Psi(\boldsymbol{k}^*) \delta_{(\boldsymbol{k}^*)} &\leftrightarrow \Psi = \sum_{\boldsymbol{k}^*} \Psi(\boldsymbol{k}^*) \mathbf{v}_{\boldsymbol{k}^*}. \end{aligned}$$

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:

$$\begin{aligned} W_{\mathbf{N}} &\cong L(\Lambda_{\mathbf{B}}/\Lambda_{\mathbf{A}}) \cong L(\mathbb{Z}^n/\mathbf{N}\mathbb{Z}^n) \\ W_{\mathbf{N}}^* &\cong L(\Lambda_{\mathbf{A}}^*/\Lambda_{\mathbf{B}}^*) \cong L(\mathbb{Z}^n/\mathbf{N}^T \mathbb{Z}^n) \end{aligned}$$

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

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

$$\begin{aligned} (\varphi, \psi)_W &= \sum_{\boldsymbol{k}} \overline{\varphi(\boldsymbol{k})} \psi(\boldsymbol{k}) \\ (\Phi, \Psi)_{W^*} &= \sum_{\boldsymbol{k}^*} \overline{\Phi(\boldsymbol{k}^*)} \Psi(\boldsymbol{k}^*), \end{aligned}$$

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.

1.3. FOURIER TRANSFORMS IN CRYSTALLOGRAPHY

1.3.2.7.4. Matrix representation of the discrete Fourier transform (DFT)

By virtue of definitions (i) and (ii),

$$\begin{aligned}\mathcal{F}(\mathbf{N})\mathbf{v}_{k^*} &= \frac{1}{|\det \mathbf{N}|} \sum_k \exp[-2\pi i k^* \cdot (\mathbf{N}^{-1}k)] \mathbf{u}_k \\ \tilde{\mathcal{F}}(\mathbf{N})\mathbf{u}_k &= \sum_{k^*} \exp[+2\pi i k^* \cdot (\mathbf{N}^{-1}k)] \mathbf{v}_{k^*}\end{aligned}$$

so that $\mathcal{F}(\mathbf{N})$ and $\tilde{\mathcal{F}}(\mathbf{N})$ may be represented, in the canonical bases of $W_{\mathbf{N}}$ and $W_{\mathbf{N}}^*$, by the following matrices:

$$\begin{aligned}[\mathcal{F}(\mathbf{N})]_{kk^*} &= \frac{1}{|\det \mathbf{N}|} \exp[-2\pi i k^* \cdot (\mathbf{N}^{-1}k)] \\ [\tilde{\mathcal{F}}(\mathbf{N})]_{k^*k} &= \exp[+2\pi i k^* \cdot (\mathbf{N}^{-1}k)].\end{aligned}$$

When \mathbf{N} is symmetric, $\mathbb{Z}^n/\mathbf{N}\mathbb{Z}^n$ and $\mathbb{Z}^n/\mathbf{N}^T\mathbb{Z}^n$ may be identified in a natural manner, and the above matrices are symmetric.

When \mathbf{N} is diagonal, say $\mathbf{N} = \text{diag}(\nu_1, \nu_2, \dots, \nu_n)$, then the tensor product structure of the full multidimensional Fourier transform (Section 1.3.2.4.2.4)

$$\mathcal{F}_{\mathbf{x}} = \mathcal{F}_{x_1} \otimes \mathcal{F}_{x_2} \otimes \dots \otimes \mathcal{F}_{x_n}$$

gives rise to a tensor product structure for the DFT matrices. The tensor product of matrices is defined as follows:

$$\mathbf{A} \otimes \mathbf{B} = \begin{pmatrix} a_{11}\mathbf{B} & \dots & a_{1n}\mathbf{B} \\ \vdots & & \vdots \\ a_{n1}\mathbf{B} & \dots & a_{nn}\mathbf{B} \end{pmatrix}.$$

Let the index vectors k and k^* be ordered in the same way as the elements in a Fortran array, e.g. for k with k_1 increasing fastest, k_2 next fastest, \dots , k_n slowest; then

$$\mathcal{F}(\mathbf{N}) = \mathcal{F}(\nu_1) \otimes \mathcal{F}(\nu_2) \otimes \dots \otimes \mathcal{F}(\nu_n),$$

where

$$[\mathcal{F}(\nu_j)]_{k_j, k_j^*} = \frac{1}{\nu_j} \exp\left(-2\pi i \frac{k_j^* k_j}{\nu_j}\right),$$

and

$$\tilde{\mathcal{F}}(\mathbf{N}) = \tilde{\mathcal{F}}(\nu_1) \otimes \tilde{\mathcal{F}}(\nu_2) \otimes \dots \otimes \tilde{\mathcal{F}}(\nu_n),$$

where

$$[\tilde{\mathcal{F}}(\nu_j)]_{k_j^*, k_j} = \exp\left(+2\pi i \frac{k_j^* k_j}{\nu_j}\right).$$

1.3.2.7.5. Properties of the discrete Fourier transform

The DFT inherits most of the properties of the Fourier transforms, but with certain numerical factors ('Jacobians') due to the transition from continuous to discrete measure.

(1) *Linearity* is obvious.

(2) *Shift property.* If $(\tau_a \psi)(k) = \psi(k - a)$ and $(\tau_a \Psi)(k^*) = \Psi(k^* - a^*)$, where subtraction takes place by modular vector arithmetic in $\mathbb{Z}^n/\mathbf{N}\mathbb{Z}^n$ and $\mathbb{Z}^n/\mathbf{N}^T\mathbb{Z}^n$, respectively, then the following identities hold:

$$\begin{aligned}\tilde{\mathcal{F}}(\mathbf{N})[\tau_k \psi](k^*) &= \exp[+2\pi i k^* \cdot (\mathbf{N}^{-1}k)] \tilde{\mathcal{F}}(\mathbf{N})[\psi](k^*) \\ \mathcal{F}(\mathbf{N})[\tau_{k^*} \Psi](k) &= \exp[-2\pi i k^* \cdot (\mathbf{N}^{-1}k)] \mathcal{F}(\mathbf{N})[\Psi](k).\end{aligned}$$

(3) *Differentiation identities.* Let vectors ψ and Ψ be constructed from $\varphi^0 \in \mathcal{E}(\mathbb{R}^n)$ as in Section 1.3.2.7.3, hence be related by the DFT. If $D^{\mathbf{p}}\psi$ designates the vector of sample values of $D_{\mathbf{x}}^{\mathbf{p}}\varphi^0$ at the points of $\Lambda_{\mathbf{B}}/\Lambda_{\mathbf{A}}$, and $D^{\mathbf{p}}\Psi$ the vector of values of $D_{\xi}^{\mathbf{p}}\Phi^0$ at points of

$\Lambda_{\mathbf{A}}^*/\Lambda_{\mathbf{B}}^*$, then for all multi-indices $\mathbf{p} = (p_1, p_2, \dots, p_n)$

$$\begin{aligned}(D^{\mathbf{p}}\psi)(k) &= \tilde{\mathcal{F}}(\mathbf{N})[(+2\pi i k^*)^{\mathbf{p}}\Psi](k) \\ (D^{\mathbf{p}}\Psi)(k^*) &= \mathcal{F}(\mathbf{N})[(-2\pi i k)^{\mathbf{p}}\psi](k^*)\end{aligned}$$

or equivalently

$$\begin{aligned}\tilde{\mathcal{F}}(\mathbf{N})[D^{\mathbf{p}}\psi](k^*) &= (+2\pi i k^*)^{\mathbf{p}}\Psi(k^*) \\ \mathcal{F}(\mathbf{N})[D^{\mathbf{p}}\Psi](k) &= (-2\pi i k)^{\mathbf{p}}\psi(k).\end{aligned}$$

(4) *Convolution property.* Let $\varphi \in W_{\mathbf{N}}$ and $\Phi \in W_{\mathbf{N}}^*$ (respectively ψ and Ψ) be related by the DFT, and define

$$\begin{aligned}(\varphi * \psi)(k) &= \sum_{k' \in \mathbb{Z}^n/\mathbf{N}\mathbb{Z}^n} \varphi(k') \psi(k - k') \\ (\Phi * \Psi)(k^*) &= \sum_{k' \in \mathbb{Z}^n/\mathbf{N}^T\mathbb{Z}^n} \Phi(k') \Psi(k^* - k').\end{aligned}$$

Then

$$\begin{aligned}\tilde{\mathcal{F}}(\mathbf{N})[\Phi * \Psi](k) &= |\det \mathbf{N}| \varphi(k) \psi(k) \\ \mathcal{F}(\mathbf{N})[\varphi * \psi](k^*) &= \Phi(k^*) \Psi(k^*)\end{aligned}$$

and

$$\begin{aligned}\tilde{\mathcal{F}}(\mathbf{N})[\varphi \times \psi](k^*) &= \frac{1}{|\det \mathbf{N}|} (\Phi * \Psi)(k^*) \\ \mathcal{F}(\mathbf{N})[\Phi \times \Psi](k) &= (\varphi * \psi)(k).\end{aligned}$$

Since addition on $\mathbb{Z}^n/\mathbf{N}\mathbb{Z}^n$ and $\mathbb{Z}^n/\mathbf{N}^T\mathbb{Z}^n$ is modular, this type of convolution is called *cyclic convolution*.

(5) *Parseval/Plancherel property.* If $\varphi, \psi, \Phi, \Psi$ are as above, then

$$\begin{aligned}(\mathcal{F}(\mathbf{N})[\Phi], \mathcal{F}(\mathbf{N})[\Psi])_W &= \frac{1}{|\det \mathbf{N}|} (\Phi, \Psi)_{W^*} \\ (\tilde{\mathcal{F}}(\mathbf{N})[\varphi], \tilde{\mathcal{F}}(\mathbf{N})[\psi])_W &= \frac{1}{|\det \mathbf{N}|} (\varphi, \psi)_W.\end{aligned}$$

(6) *Period 4.* When \mathbf{N} is symmetric, so that the ranges of indices k and k^* can be identified, it makes sense to speak of powers of $\mathcal{F}(\mathbf{N})$ and $\tilde{\mathcal{F}}(\mathbf{N})$. Then the 'standardized' matrices $(1/|\det \mathbf{N}|^{1/2})\mathcal{F}(\mathbf{N})$ and $(1/|\det \mathbf{N}|^{1/2})\tilde{\mathcal{F}}(\mathbf{N})$ are *unitary* matrices whose fourth power is the identity matrix (Section 1.3.2.4.3.4); their eigenvalues are therefore ± 1 and $\pm i$.

1.3.3. Numerical computation of the discrete Fourier transform

1.3.3.1. Introduction

The Fourier transformation's most remarkable property is undoubtedly that of turning convolution into multiplication. As distribution theory has shown, other valuable properties – such as the shift property, the conversion of differentiation into multiplication by monomials, and the duality between periodicity and sampling – are special instances of the convolution theorem.

This property is exploited in many areas of applied mathematics and engineering (Campbell & Foster, 1948; Sneddon, 1951; Champeney, 1973; Bracewell, 1986). For example, the passing of a signal through a linear filter, which results in its being convolved with the response of the filter to a δ -function 'impulse', may be modelled as a multiplication of the signal's transform by the transform of the impulse response (also called transfer function). Similarly, the solution of systems of partial differential equations may be turned by Fourier transformation into a division problem for distributions. In both cases, the formulations obtained after Fourier transformation are considerably simpler than the initial ones, and lend themselves to constructive solution techniques.