

1.3. FOURIER TRANSFORMS IN CRYSTALLOGRAPHY

standard n -torus \mathbb{R}^n/Λ . The correspondence to crystallographic terminology is that ‘standard’ coordinates over the standard 3-torus $\mathbb{R}^3/\mathbb{Z}^3$ are called ‘fractional’ coordinates over the unit cell; while Cartesian coordinates, e.g. in ångströms, constitute a set of non-standard coordinates.

Finally, we will denote by I the unit cube $[0, 1]^n$ and by C_ε the subset

$$C_\varepsilon = \{\mathbf{x} \in \mathbb{R}^n \mid |x_j| < \varepsilon \text{ for all } j = 1, \dots, n\}.$$

1.3.2.6.2. \mathbb{Z}^n -periodic distributions in \mathbb{R}^n

A distribution $T \in \mathcal{D}'(\mathbb{R}^n)$ is called *periodic with period lattice* \mathbb{Z}^n (or \mathbb{Z}^n -periodic) if $\tau_{\mathbf{m}}T = T$ for all $\mathbf{m} \in \mathbb{Z}^n$ (in crystallography the period lattice is the *direct* lattice).

Given a distribution with compact support $T^0 \in \mathcal{E}'(\mathbb{R}^n)$, then $T = \sum_{\mathbf{m} \in \mathbb{Z}^n} \tau_{\mathbf{m}}T^0$ is a \mathbb{Z}^n -periodic distribution. Note that we may write $T = r * T^0$, where $r = \sum_{\mathbf{m} \in \mathbb{Z}^n} \delta_{(\mathbf{m})}$ consists of Dirac δ 's at all nodes of the period lattice \mathbb{Z}^n .

Conversely, any \mathbb{Z}^n -periodic distribution T may be written as $r * T^0$ for some $T^0 \in \mathcal{E}'$. To retrieve such a ‘motif’ T^0 from T , a function ψ will be constructed in such a way that $\psi \in \mathcal{D}$ (hence has compact support) and $r * \psi = 1$; then $T^0 = \psi T$. Indicator functions (Section 1.3.2.2) such as χ_1 or $\chi_{C_{1/2}}$ cannot be used directly, since they are discontinuous; but regularized versions of them may be constructed by convolution (see Section 1.3.2.3.9.7) as $\psi_0 = \chi_{C_\varepsilon} * \theta_\eta$, with ε and η such that $\psi_0(\mathbf{x}) = 1$ on $C_{1/2}$ and $\psi_0(\mathbf{x}) = 0$ outside $C_{3/4}$. Then the function

$$\psi = \frac{\psi_0}{\sum_{\mathbf{m} \in \mathbb{Z}^n} \tau_{\mathbf{m}}\psi_0}$$

has the desired property. The sum in the denominator contains at most 2^n non-zero terms at any given point \mathbf{x} and acts as a smoothly varying ‘multiplicity correction’.

1.3.2.6.3. Identification with distributions over $\mathbb{R}^n/\mathbb{Z}^n$

Throughout this section, ‘periodic’ will mean ‘ \mathbb{Z}^n -periodic’.

Let $s \in \mathbb{R}$, and let $[s]$ denote the largest integer $\leq s$. For $x = (x_1, \dots, x_n) \in \mathbb{R}^n$, let $\tilde{\mathbf{x}}$ be the unique vector $(\tilde{x}_1, \dots, \tilde{x}_n)$ with $\tilde{x}_j = x_j - [x_j]$. If $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$, then $\tilde{\mathbf{x}} = \tilde{\mathbf{y}}$ if and only if $\mathbf{x} - \mathbf{y} \in \mathbb{Z}^n$. The image of the map $\mathbf{x} \mapsto \tilde{\mathbf{x}}$ is thus \mathbb{R}^n modulo \mathbb{Z}^n , or $\mathbb{R}^n/\mathbb{Z}^n$.

If f is a periodic function over \mathbb{R}^n , then $\tilde{\mathbf{x}} = \tilde{\mathbf{y}}$ implies $f(\mathbf{x}) = f(\mathbf{y})$; we may thus define a function \tilde{f} over $\mathbb{R}^n/\mathbb{Z}^n$ by putting $\tilde{f}(\tilde{\mathbf{x}}) = f(\mathbf{x})$ for any $\mathbf{x} \in \mathbb{R}^n$ such that $\mathbf{x} - \tilde{\mathbf{x}} \in \mathbb{Z}^n$. Conversely, if \tilde{f} is a function over $\mathbb{R}^n/\mathbb{Z}^n$, then we may define a function f over \mathbb{R}^n by putting $f(\mathbf{x}) = \tilde{f}(\tilde{\mathbf{x}})$, and f will be periodic. Periodic functions over \mathbb{R}^n may thus be identified with functions over $\mathbb{R}^n/\mathbb{Z}^n$, and this identification preserves the notions of convergence, local summability and differentiability.

Given $\varphi^0 \in \mathcal{D}'(\mathbb{R}^n)$, we may define

$$\varphi(\mathbf{x}) = \sum_{\mathbf{m} \in \mathbb{Z}^n} (\tau_{\mathbf{m}}\varphi^0)(\mathbf{x})$$

since the sum only contains finitely many non-zero terms; φ is periodic, and $\tilde{\varphi} \in \mathcal{D}'(\mathbb{R}^n/\mathbb{Z}^n)$. Conversely, if $\tilde{\varphi} \in \mathcal{D}'(\mathbb{R}^n/\mathbb{Z}^n)$ we may define $\varphi \in \mathcal{E}'(\mathbb{R}^n)$ periodic by $\varphi(\mathbf{x}) = \tilde{\varphi}(\tilde{\mathbf{x}})$, and $\varphi^0 \in \mathcal{D}'(\mathbb{R}^n)$ by putting $\varphi^0 = \psi\varphi$ with ψ constructed as above.

By transposition, a distribution $\tilde{T} \in \mathcal{D}'(\mathbb{R}^n/\mathbb{Z}^n)$ defines a unique periodic distribution $T \in \mathcal{D}'(\mathbb{R}^n)$ by $\langle T, \varphi^0 \rangle = \langle \tilde{T}, \tilde{\varphi} \rangle$; conversely, $T \in \mathcal{D}'(\mathbb{R}^n)$ periodic defines uniquely $\tilde{T} \in \mathcal{D}'(\mathbb{R}^n/\mathbb{Z}^n)$ by $\langle \tilde{T}, \tilde{\varphi} \rangle = \langle T, \varphi^0 \rangle$.

We may therefore identify \mathbb{Z}^n -periodic distributions over \mathbb{R}^n with distributions over $\mathbb{R}^n/\mathbb{Z}^n$. We will, however, use mostly the former

presentation, as it is more closely related to the crystallographer’s perception of periodicity (see Section 1.3.4.1).

1.3.2.6.4. Fourier transforms of periodic distributions

The content of this section is perhaps the central result in the relation between Fourier theory and crystallography (Section 1.3.4.2.1.1).

Let $T = r * T^0$ with r defined as in Section 1.3.2.6.2. Then $r \in \mathcal{D}'$, $T^0 \in \mathcal{E}'$ hence $T^0 \in \mathcal{O}'_C$, so that $T \in \mathcal{D}'$: \mathbb{Z}^n -periodic distributions are tempered, hence have a Fourier transform. The convolution theorem (Section 1.3.2.5.8) is applicable, giving:

$$\mathcal{F}[T] = \mathcal{F}[r] \times \mathcal{F}[T^0]$$

and similarly for $\tilde{\mathcal{F}}$.

Since $\mathcal{F}[\delta_{(\mathbf{m})}](\xi) = \exp(-2\pi i \xi \cdot \mathbf{m})$, formally

$$\mathcal{F}[r]_\xi = \sum_{\mathbf{m} \in \mathbb{Z}^n} \exp(-2\pi i \xi \cdot \mathbf{m}) = Q,$$

say.

It is readily shown that Q is tempered and periodic, so that $Q = \sum_{\mu \in \mathbb{Z}^n} \tau_\mu(\psi Q)$, while the periodicity of r implies that

$$[\exp(-2\pi i \xi_j) - 1]\psi Q = 0, \quad j = 1, \dots, n.$$

Since the first factors have single isolated zeros at $\xi_j = 0$ in $C_{3/4}$, $\psi Q = c\delta$ (see Section 1.3.2.3.9.4) and hence by periodicity $Q = cr$; convoluting with χ_{C_1} shows that $c = 1$. Thus we have the fundamental result:

$$\boxed{\mathcal{F}[r] = r}$$

so that

$$\mathcal{F}[T] = r \times \mathcal{F}[T^0];$$

i.e., according to Section 1.3.2.3.9.3,

$$\mathcal{F}[T]_\xi = \sum_{\mu \in \mathbb{Z}^n} \mathcal{F}[T^0](\mu) \times \delta_{(\mu)}.$$

The right-hand side is a *weighted* lattice distribution, whose nodes $\mu \in \mathbb{Z}^n$ are weighted by the *sample values* $\mathcal{F}[T^0](\mu)$ of the transform of the motif T^0 at those nodes. Since $T^0 \in \mathcal{E}'$, the latter values may be written

$$\mathcal{F}[T^0](\mu) = \langle T^0_x, \exp(-2\pi i \mu \cdot \mathbf{x}) \rangle.$$

By the structure theorem for distributions with compact support (Section 1.3.2.3.9.7), T^0 is a derivative of finite order of a continuous function; therefore, from Section 1.3.2.4.2.8 and Section 1.3.2.5.8, $\mathcal{F}[T^0](\mu)$ grows at most polynomially as $\|\mu\| \rightarrow \infty$ (see also Section 1.3.2.6.10.3 about this property). Conversely, let $W = \sum_{\mu \in \mathbb{Z}^n} w_\mu \delta_{(\mu)}$ be a weighted lattice distribution such that the weights w_μ grow at most polynomially as $\|\mu\| \rightarrow \infty$. Then W is a tempered distribution, whose Fourier cotransform $T_x = \sum_{\mu \in \mathbb{Z}^n} w_\mu \exp(+2\pi i \mu \cdot \mathbf{x})$ is periodic. If T is now written as $r * T^0$ for some $T^0 \in \mathcal{E}'$, then by the reciprocity theorem

$$w_\mu = \mathcal{F}[T^0](\mu) = \langle T_x, \exp(-2\pi i \mu \cdot \mathbf{x}) \rangle.$$

Although the choice of T^0 is not unique, and need not yield back the same motif as may have been used to build T initially, different choices of T^0 will lead to the same coefficients w_μ because of the periodicity of $\exp(-2\pi i \mu \cdot \mathbf{x})$.

The Fourier transformation thus establishes a duality between periodic distributions and weighted lattice distributions. The pair of relations