International Tables for Crystallography (2006). Vol. B, Section 1.3.2.6.3, p. 41.

standard n-torus $\mathbb{R}^n/\Lambda$. 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

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

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

A distribution $T \in \mathscr{D}'(\mathbb{R}^n)$ 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 $T^0 \in \mathscr{E}'(\mathbb{R}^n)$, 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 $T^0 \in \mathscr{E}'$. To retrieve such a 'motif' T^0 from T, a function ψ will be constructed in such a way that $\psi \in \mathscr{D}$ (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 $x = (x_1, \ldots, x_n) \in \mathbb{R}^n$, let $\tilde{\mathbf{x}}$ be the unique vector $(\tilde{x}_1, \ldots, \tilde{x}_n)$ 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 $\mathbf{x} \longmapsto \tilde{\mathbf{x}}$ 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 $\varphi^0 \in \mathscr{D}(\mathbb{R}^n)$, 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 $\tilde{\varphi} \in \mathscr{D}(\mathbb{R}^n/\mathbb{Z}^n)$. Conversely, if $\tilde{\varphi} \in \mathscr{D}(\mathbb{R}^n/\mathbb{Z}^n)$ we may define $\varphi \in \mathscr{E}(\mathbb{R}^n)$ periodic by $\varphi(\mathbf{x}) = \tilde{\varphi}(\tilde{\mathbf{x}})$, and $\varphi^0 \in \mathscr{D}(\mathbb{R}^n)$ by putting $\varphi^0 = \psi\varphi$ with ψ constructed as above.

By transposition, a distribution $\tilde{T} \in \mathscr{D}'(\mathbb{R}^n/\mathbb{Z}^n)$ defines a unique periodic distribution $T \in \mathscr{D}'(\mathbb{R}^n)$ by $\langle T, \varphi^0\rangle = \langle \tilde{T}, \tilde{\varphi}\rangle$; conversely, $T \in \mathscr{D}'(\mathbb{R}^n)$ periodic defines uniquely $\tilde{T} \in \mathscr{D}'(\mathbb{R}^n/\mathbb{Z}^n)$ 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 $r \in \mathscr{S}'$, $T^0 \in \mathscr{E}'$ hence $T^0 \in \mathscr{O}'_C$, so that $T \in \mathscr{S}'$: $\mathbb{Z}^n$-periodic distributions are tempered, hence have a Fourier transform. The convolution theorem (Section 1.3.2.5.8) is applicable, giving:

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

and similarly for $\bar{\mathscr{F}}$.

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

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

say.

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

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

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:

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

so that

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

i.e., according to Section 1.3.2.3.9.3,

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

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

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

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, $\mathscr{F}[T^0](\boldsymbol{\mu})$ grows at most polynomially as $\|\boldsymbol{\mu}\| \to \infty$ (see also Section 1.3.2.6.10.3 about this property). Conversely, let $W = \sum_{\boldsymbol{\mu}\in\mathbb{Z}^n} w_{\boldsymbol{\mu}} \delta_{(\boldsymbol{\mu})}$ be a weighted lattice distribution such that the weights $w_{\boldsymbol{\mu}}$ grow at most polynomially as $\|\boldsymbol{\mu}\| \to \infty$. Then W is a tempered distribution, whose Fourier cotransform $T_{\mathbf{x}} = \sum_{\boldsymbol{\mu}\in\mathbb{Z}^n} w_{\boldsymbol{\mu}} \exp(+2\pi i \boldsymbol{\mu} \cdot \mathbf{x})$ is periodic. If T is now written as $r * T^0$ for some $T^0 \in \mathscr{E}'$, then by the reciprocity theorem

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

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 $w_{\boldsymbol{\mu}}$ because of the periodicity of $\exp(-2\pi i \boldsymbol{\mu} \cdot \mathbf{x})$.

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

references