International Tables for Crystallography (2006). Vol. B, Section 1.3.2.6.4, pp. 41–42.

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

$$\text{(i)} \qquad w_{\boldsymbol{\mu}} = \langle T^0_{\mathbf{x}}, \exp(-2\pi i \boldsymbol{\mu}\cdot\mathbf{x})\rangle$$

$$\text{(ii)} \qquad T_{\mathbf{x}} = \sum_{\boldsymbol{\mu}\in\mathbb{Z}^n} w_{\boldsymbol{\mu}} \exp(+2\pi i \boldsymbol{\mu}\cdot\mathbf{x})$$

are referred to as the *Fourier analysis* and the *Fourier synthesis* of T, respectively (there is a discrepancy between this terminology and the crystallographic one, see Section 1.3.4.2.1.1). In other words, any periodic distribution $T \in \mathscr{S}'$ may be represented by a Fourier series (ii), whose coefficients are calculated by (i). The convergence of (ii) towards T in $\mathscr{S}'$ will be investigated later (Section 1.3.2.6.10).

1.3.2.6.5. *The case of non-standard period lattices*

Let Λ denote the non-standard lattice consisting of all vectors of the form $\sum_{j=1} m_j\mathbf{a}_j$, where the m_j are rational integers and $\mathbf{a}_1, \ldots, \mathbf{a}_n$ are n linearly independent vectors in $\mathbb{R}^n$. Let R be the corresponding lattice distribution: $R = \sum_{x\in\Lambda}\delta_{(\mathbf{x})}$.

Let $\mathbf{A}$ be the non-singular $n\times n$ matrix whose successive columns are the coordinates of vectors $\mathbf{a}_1, \ldots, \mathbf{a}_n$ in the standard basis of $\mathbb{R}^n$; $\mathbf{A}$ will be called the *period matrix* of Λ, and the mapping $\mathbf{x}\longmapsto\mathbf{Ax}$ will be denoted by A. According to Section 1.3.2.3.9.5 we have

$$\langle R, \varphi\rangle = \sum_{\mathbf{m}\in\mathbb{Z}^n}\varphi(\mathbf{Am}) = \langle r, (A^{-1})^{\#}\varphi\rangle = |\det \mathbf{A}|^{-1}\langle A^{\#}r, \varphi\rangle$$

for any $\varphi\in\mathscr{S}$, and hence $R = |\det \mathbf{A}|^{-1}A^{\#}r$. By Fourier transformation, according to Section 1.3.2.5.5,

$$\mathscr{F}[R] = |\det \mathbf{A}|^{-1}\mathscr{F}[A^{\#}r] = [(\mathbf{A}^{-1})^T]^{\#}\mathscr{F}[r] = [(\mathbf{A}^{-1})^T]^{\#}r,$$

which we write:

$$\mathscr{F}[R] = |\det \mathbf{A}|^{-1}R^*$$

with

$$R^* = |\det \mathbf{A}|[(\mathbf{A}^{-1})^T]^{\#}r.$$

R^* is a lattice distribution:

$$R^* = \sum_{\boldsymbol{\mu}\in\mathbb{Z}^n}\delta_{[(\mathbf{A}^{-1})^T\boldsymbol{\mu}]} = \sum_{\boldsymbol{\xi}\in\Lambda^*}\delta_{(\boldsymbol{\xi})}$$

associated with the *reciprocal lattice* Λ^* whose basis vectors $\mathbf{a}_1^*, \ldots, \mathbf{a}_n^*$ are the columns of $(\mathbf{A}^{-1})^T$. Since the latter matrix is equal to the adjoint matrix (*i.e.* the matrix of co-factors) of $\mathbf{A}$ divided by $\det \mathbf{A}$, the components of the reciprocal basis vectors can be written down explicitly (see Section 1.3.4.2.1.1 for the crystallographic case $n = 3$).

A distribution T will be called Λ-*periodic* if $\tau_{\boldsymbol{\xi}}T = T$ for all $\boldsymbol{\xi}\in\Lambda$; as previously, T may be written $R * T^0$ for some motif distribution T^0 with compact support. By Fourier transformation,

$$\begin{aligned}\mathscr{F}[T] &= |\det \mathbf{A}|^{-1}R^*\cdot\mathscr{F}[T^0]\\ &= |\det \mathbf{A}|^{-1}\sum_{\boldsymbol{\xi}\in\Lambda^*}\mathscr{F}[T^0](\boldsymbol{\xi})\delta_{(\boldsymbol{\xi})}\\ &= |\det \mathbf{A}|^{-1}\sum_{\boldsymbol{\mu}\in\mathbb{Z}^n}\mathscr{F}[T^0][(\mathbf{A}^{-1})^T\boldsymbol{\mu}]\delta_{[(\mathbf{A}^{-1})^T\boldsymbol{\mu}]}\end{aligned}$$

so that $\mathscr{F}[T]$ is a weighted reciprocal-lattice distribution, the weight attached to node $\boldsymbol{\xi}\in\Lambda^*$ being $|\det \mathbf{A}|^{-1}$ times the value $\mathscr{F}[T^0](\boldsymbol{\xi})$ of the Fourier transform of the motif T^0.

This result may be further simplified if T and its motif T^0 are referred to the standard period lattice $\mathbb{Z}^n$ by defining t and t^0 so that $T = A^{\#}t$, $T^0 = A^{\#}t^0$, $t = r * t^0$. Then

$$\mathscr{F}[T^0](\boldsymbol{\xi}) = |\det \mathbf{A}|\mathscr{F}[t^0](\mathbf{A}^T\boldsymbol{\xi}),$$

hence

$$\mathscr{F}[T^0][(\mathbf{A}^{-1})^T\boldsymbol{\mu}] = |\det \mathbf{A}|\mathscr{F}[t^0](\boldsymbol{\mu}),$$

so that

$$\mathscr{F}[T] = \sum_{\boldsymbol{\mu}\in\mathbb{Z}^n}\mathscr{F}[t^0](\boldsymbol{\mu})\delta_{[(\mathbf{A}^{-1})^T\boldsymbol{\mu}]}$$

in non-standard coordinates, while

$$\mathscr{F}[t] = \sum_{\boldsymbol{\mu}\in\mathbb{Z}^n}\mathscr{F}[t^0](\boldsymbol{\mu})\delta_{(\boldsymbol{\mu})}$$

in standard coordinates.

The reciprocity theorem may then be written:

$$\text{(iii)} \qquad W_{\boldsymbol{\xi}} = |\det \mathbf{A}|^{-1}\langle T^0_{\mathbf{x}}, \exp(-2\pi i\boldsymbol{\xi}\cdot\mathbf{x})\rangle, \quad \boldsymbol{\xi}\in\boldsymbol{\Lambda}^*$$

$$\text{(iv)} \qquad T_{\mathbf{x}} = \sum_{\boldsymbol{\xi}\in\Lambda^*} W_{\boldsymbol{\xi}}\exp(+2\pi i\boldsymbol{\xi}\cdot\mathbf{x})$$

in non-standard coordinates, or equivalently:

$$\text{(v)} \qquad w_{\boldsymbol{\mu}} = \langle t^0_{\mathbf{x}}, \exp(-2\pi i\boldsymbol{\mu}\cdot\mathbf{x})\rangle, \quad \boldsymbol{\mu}\in\mathbb{Z}^n$$

$$\text{(vi)} \qquad t_{\mathbf{x}} = \sum_{\boldsymbol{\mu}\in\mathbb{Z}^n} w_{\boldsymbol{\mu}}\exp(+2\pi i\boldsymbol{\mu}\cdot\mathbf{x})$$

in standard coordinates. It gives an n-dimensional Fourier series representation for any periodic distribution over $\mathbb{R}^n$. The convergence of such series in $\mathscr{S}'(\mathbb{R}^n)$ will be examined in Section 1.3.2.6.10.

1.3.2.6.6. *Duality between periodization and sampling*

Let T^0 be a distribution with compact support (the 'motif'). Its Fourier transform $\bar{\mathscr{F}}[T^0]$ is analytic (Section 1.3.2.5.4) and may thus be used as a multiplier.

We may rephrase the preceding results as follows:

(i) if T^0 is 'periodized by R' to give $R * T^0$, then $\bar{\mathscr{F}}[T^0]$ is 'sampled by R^*' to give $|\det \mathbf{A}|^{-1}R^*\cdot\bar{\mathscr{F}}[T^0]$;

(ii) if $\bar{\mathscr{F}}[T^0]$ is 'sampled by R^*' to give $R^*\cdot\bar{\mathscr{F}}[T^0]$, then T^0 is 'periodized by R' to give $|\det \mathbf{A}|R * T^0$.

Thus the Fourier transformation establishes a duality between the periodization of a distribution by a period lattice Λ and the sampling of its transform at the nodes of lattice Λ^* reciprocal to Λ. This is a particular instance of the convolution theorem of Section 1.3.2.5.8.

At this point it is traditional to break the symmetry between $\mathscr{F}$ and $\bar{\mathscr{F}}$ which distribution theory has enabled us to preserve even in the presence of periodicity, and to perform two distinct identifications:

(i) a Λ-periodic distribution T will be handled as a distribution $\tilde{T}$ on $\mathbb{R}^n/\Lambda$, was done in Section 1.3.2.6.3;

(ii) a weighted lattice distribution $W = \sum_{\boldsymbol{\mu}\in\mathbb{Z}^n}W_{\boldsymbol{\mu}}\delta_{[(\mathbf{A}^{-1})^T\boldsymbol{\mu}]}$ will be identified with the collection $\{W_{\boldsymbol{\mu}}|\boldsymbol{\mu}\in\mathbb{Z}^n\}$ of its n-tuply indexed coefficients.

1.3.2.6.7. *The Poisson summation formula*

Let $\varphi\in\mathscr{S}$, so that $\mathscr{F}[\varphi]\in\mathscr{S}$. Let R be the lattice distribution associated to lattice Λ, with period matrix $\mathbf{A}$, and let R^* be associated to the reciprocal lattice Λ^*. Then we may write:

$$\begin{aligned}\langle R, \varphi\rangle &= \langle R, \bar{\mathscr{F}}[\mathscr{F}[\varphi]]\rangle\\ &= \langle\bar{\mathscr{F}}[R], \mathscr{F}[\varphi]\rangle\\ &= |\det \mathbf{A}|^{-1}\langle R^*, \mathscr{F}[\varphi]\rangle\end{aligned}$$

i.e.

references