International Tables for Crystallography (2006). Vol. B, Section 1.3.2.6.1, pp. 40–41.

$$\mathscr{F}[\delta_{\mathbf{x}}^{(\mathbf{m})}]_{\boldsymbol{\xi}} = (2\pi i\boldsymbol{\xi})^{\mathbf{m}}, \quad \mathscr{F}[\mathbf{x}^{\mathbf{m}}]_{\boldsymbol{\xi}} = (-2\pi i)^{-|\mathbf{m}|}\delta_{\boldsymbol{\xi}}^{(\mathbf{m})};$$
$$\mathscr{F}[\delta_{\mathbf{a}}]_{\boldsymbol{\xi}} = \exp(-2\pi i\mathbf{a}\cdot\boldsymbol{\xi}), \quad \mathscr{F}[\exp(2\pi i\boldsymbol{\alpha}\cdot\mathbf{x})]_{\boldsymbol{\xi}} = \delta_{\boldsymbol{\alpha}},$$

with analogous relations for $\bar{\mathscr{F}}$, i becoming $-i$. Thus derivatives of δ are mapped to monomials (and *vice versa*), while translates of δ are mapped to 'phase factors' (and *vice versa*).

1.3.2.5.7. *Reciprocity theorem*

The previous results now allow a self-contained and rigorous proof of the reciprocity theorem between $\mathscr{F}$ and $\bar{\mathscr{F}}$ to be given, whereas in traditional settings (*i.e.* in L^1 and L^2) the implicit handling of δ through a limiting process is always the sticking point.

Reciprocity is first established in $\mathscr{S}$ as follows:

$$\begin{aligned}\bar{\mathscr{F}}[\mathscr{F}[\varphi]](\mathbf{x}) &= \int_{\mathbb{R}^n} \mathscr{F}[\varphi](\boldsymbol{\xi})\exp(2\pi i\boldsymbol{\xi}\cdot\mathbf{x})\,\mathrm{d}^n\boldsymbol{\xi}\\ &= \int_{\mathbb{R}^n} \mathscr{F}[\tau_{-\mathbf{x}}\varphi](\boldsymbol{\xi})\,\mathrm{d}^n\boldsymbol{\xi}\\ &= \langle 1, \mathscr{F}[\tau_{-\mathbf{x}}\varphi]\rangle\\ &= \langle \mathscr{F}[1], \tau_{-\mathbf{x}}\varphi\rangle\\ &= \langle \tau_{\mathbf{x}}\delta, \varphi\rangle\\ &= \varphi(\mathbf{x})\end{aligned}$$

and similarly

$$\mathscr{F}[\bar{\mathscr{F}}[\varphi]](\mathbf{x}) = \varphi(\mathbf{x}).$$

The reciprocity theorem is then proved in $\mathscr{S}'$ by transposition:

$$\bar{\mathscr{F}}[\mathscr{F}[T]] = \mathscr{F}[\bar{\mathscr{F}}[T]] = T \quad \text{for all } T \in \mathscr{S}'.$$

Thus the Fourier cotransformation $\bar{\mathscr{F}}$ in $\mathscr{S}'$ may legitimately be called the 'inverse Fourier transformation'.

The method of Section 1.3.2.4.3 may then be used to show that $\mathscr{F}$ and $\bar{\mathscr{F}}$ both have period 4 in $\mathscr{S}'$.

1.3.2.5.8. *Multiplication and convolution*

Multiplier functions $\alpha(\mathbf{x})$ for tempered distributions must be infinitely differentiable, as for ordinary distributions; furthermore, they must grow sufficiently slowly as $\|x\| \to \infty$ to ensure that $\alpha\varphi \in \mathscr{S}$ for all $\varphi \in \mathscr{S}$ and that the map $\varphi \longmapsto \alpha\varphi$ is continuous for the topology of $\mathscr{S}$. This leads to choosing for multipliers the subspace $\mathscr{O}_M$ consisting of functions $\alpha \in \mathscr{E}$ *of polynomial growth*. It can be shown that if f is in $\mathscr{O}_M$, then the associated distribution T_f is in $\mathscr{S}'$ (*i.e.* is a tempered distribution); and that conversely if T is in $\mathscr{S}'$, $\mu * T$ is in $\mathscr{O}_M$ for all $\mu \in \mathscr{D}$.

Corresponding restrictions must be imposed to define the space $\mathscr{O}'_C$ of those distributions T whose convolution $S * T$ with a tempered distribution S is still a tempered distribution: T must be such that, for all $\varphi \in \mathscr{S}$, $\theta(\mathbf{x}) = \langle T_{\mathbf{y}}, \varphi(\mathbf{x}+\mathbf{y})\rangle$ is in $\mathscr{S}$; and such that the map $\varphi \longmapsto \theta$ be continuous for the topology of $\mathscr{S}$. This implies that S is 'rapidly decreasing'. It can be shown that if f is in $\mathscr{S}$, then the associated distribution T_f is in $\mathscr{O}'_C$; and that conversely if T is in $\mathscr{O}'_C$, $\mu * T$ is in $\mathscr{S}$ for all $\mu \in \mathscr{D}$.

The two spaces $\mathscr{O}_M$ and $\mathscr{O}'_C$ are mapped into each other by the Fourier transformation

$$\begin{aligned}\mathscr{F}(\mathscr{O}_M) &= \bar{\mathscr{F}}(\mathscr{O}_M) = \mathscr{O}'_C\\ \mathscr{F}(\mathscr{O}'_C) &= \bar{\mathscr{F}}(\mathscr{O}'_C) = \mathscr{O}_M\end{aligned}$$

and the convolution theorem takes the form

$$\begin{aligned}\mathscr{F}[\alpha S] &= \mathscr{F}[\alpha] * \mathscr{F}[S] \quad S \in \mathscr{S}', \alpha \in \mathscr{O}_M, \mathscr{F}[\alpha] \in \mathscr{O}'_C;\\ \mathscr{F}[S * T] &= \mathscr{F}[S] \times \mathscr{F}[T] \quad S \in \mathscr{S}', T \in \mathscr{O}'_C, \mathscr{F}[T] \in \mathscr{O}_M.\end{aligned}$$

The same identities hold for $\bar{\mathscr{F}}$. Taken together with the reciprocity theorem, these show that $\mathscr{F}$ and $\bar{\mathscr{F}}$ establish mutually inverse isomorphisms between $\mathscr{O}_M$ and $\mathscr{O}'_C$, and exchange multiplication for convolution in $\mathscr{S}'$.

It may be noticed that most of the basic properties of $\mathscr{F}$ and $\bar{\mathscr{F}}$ may be deduced from this theorem and from the properties of δ. Differentiation operators $D^{\mathbf{m}}$ and translation operators $\tau_{\mathbf{a}}$ are convolutions with $D^{\mathbf{m}}\delta$ and $\tau_{\mathbf{a}}\delta$; they are turned, respectively, into multiplication by monomials $(\pm 2\pi i\boldsymbol{\xi})^{\mathbf{m}}$ (the transforms of $D^{\mathbf{m}}\delta$) or by phase factors $\exp(\pm 2\pi i\boldsymbol{\xi}\cdot\boldsymbol{\alpha})$ (the transforms of $\tau_{\mathbf{a}}\delta$).

Another consequence of the convolution theorem is the duality established by the Fourier transformation between sections and projections of a function and its transform. For instance, in $\mathbb{R}^3$, the *projection* of $f(x, y, z)$ on the x, y plane along the z axis may be written

$$(\delta_x \otimes \delta_y \otimes 1_z) * f;$$

its Fourier transform is then

$$(1_\xi \otimes 1_\eta \otimes \delta_\zeta) \times \mathscr{F}[f],$$

which is the *section* of $\mathscr{F}[f]$ by the plane $\zeta = 0$, orthogonal to the z axis used for projection. There are numerous applications of this property in crystallography (Section 1.3.4.2.1.8) and in fibre diffraction (Section 1.3.4.5.1.3).

1.3.2.5.9. L^2 *aspects, Sobolev spaces*

The special properties of $\mathscr{F}$ in the space of square-integrable functions $L^2(\mathbb{R}^n)$, such as Parseval's identity, can be accommodated within distribution theory: if $u \in L^2(\mathbb{R}^n)$, then T_u is a tempered distribution in $\mathscr{S}'$ (the map $u \longmapsto T_u$ being continuous) and it can be shown that $S = \mathscr{F}[T_u]$ is of the form S_v, where $u = \mathscr{F}[u]$ is the Fourier transform of u in $L^2(\mathbb{R}^n)$. By Plancherel's theorem, $\|u\|_2 = \|v\|_2$.

This embedding of L^2 into $\mathscr{S}'$ can be used to derive the convolution theorem for L^2. If u and v are in $L^2(\mathbb{R}^n)$, then $u * v$ can be shown to be a bounded continuous function; thus $u * v$ is not in L^2, but it is in $\mathscr{S}'$, so that its Fourier transform is a distribution, and

$$\mathscr{F}[u * v] = \mathscr{F}[u] \times \mathscr{F}[v].$$

Spaces of tempered distributions related to $L^2(\mathbb{R}^n)$ can be defined as follows. For any real s, define the Sobolev space $H_s(\mathbb{R}^n)$ to consist of all tempered distributions $S \in \mathscr{S}'(\mathbb{R}^n)$ such that

$$(1 + |\boldsymbol{\xi}|^2)^{s/2}\mathscr{F}[S]_{\boldsymbol{\xi}} \in L^2(\mathbb{R}^n).$$

These spaces play a fundamental role in the theory of partial differential equations, and in the mathematical theory of tomographic reconstruction – a subject not unrelated to the crystallographic phase problem (Natterer, 1986).

1.3.2.6. *Periodic distributions and Fourier series*

1.3.2.6.1. *Terminology*

Let $\mathbb{Z}^n$ be the subset of $\mathbb{R}^n$ consisting of those points with (signed) integer coordinates; it is an n-dimensional *lattice*, *i.e.* a free Abelian group on n generators. A particularly simple set of n generators is given by the standard basis of $\mathbb{R}^n$, and hence $\mathbb{Z}^n$ will be called the *standard lattice in* $\mathbb{R}^n$. Any other 'non-standard' n-dimensional lattice Λ in $\mathbb{R}^n$ is the image of this standard lattice by a general linear transformation.

If we identify any two points in $\mathbb{R}^n$ whose coordinates are congruent modulo $\mathbb{Z}^n$, *i.e.* differ by a vector in $\mathbb{Z}^n$, we obtain the *standard n-torus* $\mathbb{R}^n/\mathbb{Z}^n$. The latter may be viewed as $(\mathbb{R}/\mathbb{Z})^n$, *i.e.* as the Cartesian product of n circles. The same identification may be carried out modulo a non-standard lattice Λ, yielding a *non-*

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 $\le s$. 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