International Tables for Crystallography (2006). Vol. B, Section 1.3.2.6, pp. 40–45.

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

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

$$\mathscr{F}(\mathscr{O}_M) = \bar{\mathscr{F}}(\mathscr{O}_M) = \mathscr{O}'_C$$
$$\mathscr{F}(\mathscr{O}'_C) = \bar{\mathscr{F}}(\mathscr{O}'_C) = \mathscr{O}_M$$

and the convolution theorem takes the form

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

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 $\leq s$. 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.

$$\sum_{\mathbf{x}\in\Lambda}\varphi(\mathbf{x}) = |\det \mathbf{A}|^{-1} \sum_{\boldsymbol{\xi}\in\Lambda^*}\mathscr{F}[\varphi](\boldsymbol{\xi}).$$

This identity, which also holds for $\bar{\mathscr{F}}$, is called the *Poisson summation formula*. Its usefulness follows from the fact that the speed of decrease at infinity of φ and $\mathscr{F}[\varphi]$ are inversely related (Section 1.3.2.4.4.3), so that if one of the series (say, the left-hand side) is slowly convergent, the other (say, the right-hand side) will be rapidly convergent. This procedure has been used by Ewald (1921) [see also Bertaut (1952), Born & Huang (1954)] to evaluate lattice sums (Madelung constants) involved in the calculation of the internal electrostatic energy of crystals (see Chapter 3.4 in this volume on convergence acceleration techniques for crystallographic lattice sums).

When φ is a multivariate Gaussian

$$\varphi(\mathbf{x}) = G_{\mathbf{B}}(\mathbf{x}) = \exp(-\tfrac{1}{2}\mathbf{x}^T\mathbf{B}\mathbf{x}),$$

then

$$\mathscr{F}[\varphi](\boldsymbol{\xi}) = |\det\,(2\pi\mathbf{B}^{-1})|^{1/2}G_{\mathbf{B}^{-1}}(\boldsymbol{\xi}),$$

and Poisson's summation formula for a lattice with period matrix $\mathbf{A}$ reads:

$$\sum_{\mathbf{m}\in\mathbb{Z}^n} G_{\mathbf{B}}(\mathbf{A}\mathbf{m}) = |\det \mathbf{A}|^{-1}|\det\,(2\pi\mathbf{B}^{-1})|^{1/2} \times \sum_{\boldsymbol{\mu}\in\mathbb{Z}^n} G_{4\pi^2\mathbf{B}^{-1}}[(\mathbf{A}^{-1})^T\boldsymbol{\mu}]$$

or equivalently

$$\sum_{\mathbf{m}\in\mathbb{Z}^n} G_C(\mathbf{m}) = |\det\,(2\pi\mathbf{C}^{-1})|^{1/2}\sum_{\boldsymbol{\mu}\in\mathbb{Z}^n} G_{4\pi^2\mathbf{C}^{-1}}(\boldsymbol{\mu})$$

with $\mathbf{C} = \mathbf{A}^T\mathbf{B}\mathbf{A}$.

1.3.2.6.8. *Convolution of Fourier series*

Let $S = R * S^0$ and $T = R * T^0$ be two Λ-periodic distributions, the motifs S^0 and T^0 having compact support. The convolution $S * T$ does not exist, because S and T do not satisfy the support condition (Section 1.3.2.3.9.7). However, the three distributions R, S^0 and T^0 do satisfy the generalized support condition, so that their convolution is defined; then, by associativity and commutativity:

$$R * S^0 * T^0 = S * T^0 = S^0 * T.$$

By Fourier transformation and by the convolution theorem:

$$R^* \times \mathscr{F}[S^0 * T^0] = (R^* \times \mathscr{F}[S^0]) \times \mathscr{F}[T^0] = \mathscr{F}[T^0] \times (R^* \times \mathscr{F}[S^0]).$$

Let $\{U_{\boldsymbol{\xi}}\}_{\boldsymbol{\xi}\in\Lambda^*}$, $\{V_{\boldsymbol{\xi}}\}_{\boldsymbol{\xi}\in\Lambda^*}$ and $\{W_{\boldsymbol{\xi}}\}_{\boldsymbol{\xi}\in\Lambda^*}$ be the sets of Fourier coefficients associated to S, T and $S * T^0 (= S^0 * T)$, respectively. Identifying the coefficients of $\delta_{\boldsymbol{\xi}}$ for $\boldsymbol{\xi} \in \Lambda^*$ yields the forward version of the convolution theorem for Fourier series:

$$W_{\boldsymbol{\xi}} = |\det \mathbf{A}|U_{\boldsymbol{\xi}}V_{\boldsymbol{\xi}}.$$

The backward version of the theorem requires that T be infinitely differentiable. The distribution $S \times T$ is then well defined and its Fourier coefficients $\{Q_{\boldsymbol{\xi}}\}_{\boldsymbol{\xi}\in\Lambda^*}$ are given by

$$Q_{\boldsymbol{\xi}} = \sum_{\boldsymbol{\eta}\in\Lambda^*} U_{\boldsymbol{\eta}}V_{\boldsymbol{\xi}-\boldsymbol{\eta}}.$$

1.3.2.6.9. *Toeplitz forms, Szegö's theorem*

Toeplitz forms were first investigated by Toeplitz (1907, 1910, 1911*a*). They occur in connection with the 'trigonometric moment problem' (Shohat & Tamarkin, 1943; Akhiezer, 1965) and probability theory (Grenander, 1952) and play an important role in several direct approaches to the crystallographic phase problem [see Sections 1.3.4.2.1.10, 1.3.4.5.2.2(*e*)]. Many aspects of their theory and applications are presented in the book by Grenander & Szegö (1958).

1.3.2.6.9.1. *Toeplitz forms*

Let $f \in L^1(\mathbb{R}/\mathbb{Z})$ be real-valued, so that its Fourier coefficients satisfy the relations $c_{-m}(f) = \overline{c_m(f)}$. The Hermitian form in $n+1$ complex variables

$$T_n[f](\mathbf{u}) = \sum_{\mu=0}^{n}\sum_{\nu=0}^{n}\overline{u_\mu}c_{\mu-\nu}u_\nu$$

is called the nth *Toeplitz form* associated to f. It is a straightforward consequence of the convolution theorem and of Parseval's identity that $T_n[f]$ may be written:

$$T_n[f](\mathbf{u}) = \int_0^1\left|\sum_{\nu=0}^{n}u_\nu\exp(2\pi i\nu x)\right|^2 f(x)\,\mathrm{d}x.$$

1.3.2.6.9.2. *The Toeplitz–Carathéodory–Herglotz theorem*

It was shown independently by Toeplitz (1911*b*), Carathéodory (1911) and Herglotz (1911) that a function $f \in L^1$ is almost everywhere non-negative *if and only if* the Toeplitz forms $T_n[f]$ associated to f are positive semidefinite for all values of n.

This is equivalent to the infinite system of determinantal inequalities

$$D_n = \det\begin{pmatrix} c_0 & c_{-1} & \cdot & \cdot & c_{-n} \\ c_1 & c_0 & c_{-1} & \cdot & \cdot \\ \cdot & c_1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & c_{-1} \\ c_n & \cdot & \cdot & c_1 & c_0 \end{pmatrix} \geq 0 \quad \text{for all } n.$$

The D_n are called *Toeplitz determinants*. Their application to the crystallographic phase problem is described in Section 1.3.4.2.1.10.

1.3.2.6.9.3. *Asymptotic distribution of eigenvalues of Toeplitz forms*

The eigenvalues of the Hermitian form $T_n[f]$ are defined as the $n+1$ real roots of the characteristic equation $\det\{T_n[f-\lambda]\} = 0$. They will be denoted by

$$\lambda_1^{(n)}, \lambda_2^{(n)}, \ldots, \lambda_{n+1}^{(n)}.$$

It is easily shown that if $m \leq f(x) \leq M$ for all x, then $m \leq \lambda_\nu^{(n)} \leq M$ for all n and all $\nu = 1, \ldots, n+1$. As $n \to \infty$ these bounds, and the distribution of the $\lambda^{(n)}$ within these bounds, can be made more precise by introducing two new notions.

(i) *Essential bounds*: define ess inf f as the largest m such that $f(x) \geq m$ except for values of x forming a set of measure 0; and define ess sup f similarly.

(ii) *Equal distribution*. For each n, consider two sets of $n+1$ real numbers:

$$a_1^{(n)}, a_2^{(n)}, \ldots, a_{n+1}^{(n)}, \quad \text{and} \quad b_1^{(n)}, b_2^{(n)}, \ldots, b_{n+1}^{(n)}.$$

Assume that for each ν and each n, $|a_\nu^{(n)}| < K$ and $|b_\nu^{(n)}| < K$ with K independent of ν and n. The sets $\{a_\nu^{(n)}\}$ and $\{b_\nu^{(n)}\}$ are said to be equally distributed in $[-K, +K]$ if, for any function F over $[-K, +K]$,

$$\lim_{n\to\infty}\frac{1}{n+1}\sum_{\nu=1}^{n+1}[F(a_\nu^{(n)}) - F(b_\nu^{(n)})] = 0.$$

We may now state an important theorem of Szegö (1915, 1920). Let $f \in L^1$, and put $m = \text{ess inf } f$, $M = \text{ess sup } f$. If m and M are finite, then for any continuous function $F(\lambda)$ defined in the interval $[m, M]$ we have

$$\lim_{n\to\infty} \frac{1}{n+1} \sum_{\nu=1}^{n+1} F(\lambda_\nu^{(n)}) = \int_0^1 F[f(x)] \,\mathrm{d}x.$$

In other words, the eigenvalues $\lambda_\nu^{(n)}$ of the T_n and the values $f[\nu/(n+2)]$ of f on a regular subdivision of]0, 1[are equally distributed.

Further investigations into the spectra of Toeplitz matrices may be found in papers by Hartman & Wintner (1950, 1954), Kac *et al.* (1953), Widom (1965), and in the notes by Hirschman & Hughes (1977).

1.3.2.6.9.4. *Consequences of Szegö's theorem*

(i) If the λ's are ordered in ascending order, then

$$\lim_{n\to\infty} \lambda_1^{(n)} = m = \text{ess inf } f, \quad \lim_{n\to\infty} \lambda_{n+1}^{(n)} = M = \text{ess sup } f.$$

Thus, when $f \geq 0$, the condition number $\lambda_{n+1}^{(n)}/\lambda_1^{(n)}$ of $T_n[f]$ tends towards the 'essential dynamic range' M/m of f.

(ii) Let $F(\lambda) = \lambda^s$ where s is a positive integer. Then

$$\lim_{n\to\infty} \frac{1}{n+1} \sum_{\nu=1}^{n+1} [\lambda_\nu^{(n)}]^s = \int_0^1 [f(x)]^s \,\mathrm{d}x.$$

(iii) Let $m > 0$, so that $\lambda_\nu^{(n)} > 0$, and let $D_n(f) = \det T_n(f)$. Then

$$D_n(f) = \prod_{\nu=1}^{n+1} \lambda_\nu^{(n)},$$

hence

$$\log D_n(f) = \sum_{\nu=1}^{n+1} \log \lambda_\nu^{(n)}.$$

Putting $F(\lambda) = \log \lambda$, it follows that

$$\lim_{n\to\infty} [D_n(f)]^{1/(n+1)} = \exp\left\{ \int_0^1 \log f(x) \,\mathrm{d}x \right\}.$$

Further terms in this limit were obtained by Szegö (1952) and interpreted in probabilistic terms by Kac (1954).

1.3.2.6.10. *Convergence of Fourier series*

The investigation of the convergence of Fourier series and of more general trigonometric series has been the subject of intense study for over 150 years [see *e.g.* Zygmund (1976)]. It has been a constant source of new mathematical ideas and theories, being directly responsible for the birth of such fields as set theory, topology and functional analysis.

This section will briefly survey those aspects of the classical results in dimension 1 which are relevant to the practical use of Fourier series in crystallography. The books by Zygmund (1959), Tolstov (1962) and Katznelson (1968) are standard references in the field, and Dym & McKean (1972) is recommended as a stimulant.

1.3.2.6.10.1. *Classical L^1 theory*

The space $L^1(\mathbb{R}/\mathbb{Z})$ consists of (equivalence classes of) complex-valued functions f on the circle which are summable, *i.e.* for which

$$\|f\|_1 \equiv \int_0^1 |f(x)| \,\mathrm{d}x < +\infty.$$

It is a convolution algebra: If f and g are in L^1, then $f * g$ is in L^1.

The mth Fourier coefficient $c_m(f)$ of f,

$$c_m(f) = \int_0^1 f(x) \exp(-2\pi imx) \,\mathrm{d}x$$

is bounded: $|c_m(f)| \leq \|f\|_1$, and by the Riemann–Lebesgue lemma $c_m(f) \to 0$ as $m \to \infty$. By the convolution theorem, $c_m(f * g) = c_m(f)c_m(g)$.

The pth *partial sum* $S_p(f)$ of the Fourier series of f,

$$S_p(f)(x) = \sum_{|m|\leq p} c_m(f) \exp(2\pi imx),$$

may be written, by virtue of the convolution theorem, as $S_p(f) = D_p * f$, where

$$D_p(x) = \sum_{|m|\leq p} \exp(2\pi imx) = \frac{\sin[(2p+1)\pi x]}{\sin \pi x}$$

is the *Dirichlet kernel*. Because D_p comprises numerous slowly decaying oscillations, both positive and negative, $S_p(f)$ may not converge towards f in a strong sense as $p \to \infty$. Indeed, spectacular pathologies are known to exist where the partial sums, examined pointwise, diverge everywhere (Zygmund, 1959, Chapter VIII). When f is piecewise continuous, but presents isolated jumps, convergence near these jumps is marred by the *Gibbs phenomenon*: $S_p(f)$ always 'overshoots the mark' by about 9%, the area under the spurious peak tending to 0 as $p \to \infty$ but not its height [see Larmor (1934) for the history of this phenomenon].

By contrast, the *arithmetic mean* of the partial sums, also called the pth Cesàro sum,

$$C_p(f) = \frac{1}{p+1}[S_0(f) + \ldots + S_p(f)],$$

converges to f in the sense of the L^1 norm: $\|C_p(f) - f\|_1 \to 0$ as $p \to \infty$. If furthermore f is *continuous*, then the convergence is *uniform*, *i.e.* the error is bounded everywhere by a quantity which goes to 0 as $p \to \infty$. It may be shown that

$$C_p(f) = F_p * f,$$

where

$$F_p(x) = \sum_{|m|\leq p} \left(1 - \frac{|m|}{p+1}\right) \exp(2\pi imx) = \frac{1}{p+1}\left[\frac{\sin(p+1)\pi x}{\sin \pi x}\right]^2$$

is the *Fejér kernel*. F_p has over D_p the advantage of being everywhere positive, so that the Cesàro sums $C_p(f)$ of a positive function f are always positive.

The de la Vallée Poussin kernel

$$V_p(x) = 2F_{2p+1}(x) - F_p(x)$$

has a trapezoidal distribution of coefficients and is such that $c_m(V_p) = 1$ if $|m| \leq p + 1$; therefore $V_p * f$ is a trigonometric polynomial with the same Fourier coefficients as f over that range of values of m.

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):

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

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 $p \to \infty$. 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

$$\|f\|_1^2 = \left(\int_0^1 |f(x)| \times 1 \,\mathrm{d}x\right)^2 \leq \left(\int_0^1 |f(x)|^2 \,\mathrm{d}x\right)\left(\int_0^1 1^2 \,\mathrm{d}x\right) = \|f\|_2^2 \leq \infty.$$

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

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

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 $|m| \to \infty$, 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 $T_f \in \mathscr{D}'(\mathbb{R}/\mathbb{Z})$. 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 $|m| \to \infty$.

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 $\varphi \in \mathscr{E}(\mathbb{R}^n)$ be such that $\Phi = \mathscr{F}[\varphi]$ 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

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

references