International Tables for Crystallography (2006). Vol. B, Section 1.3.2.5.6, pp. 39–40.

Besides the general references to distribution theory mentioned in Section 1.3.2.3.1 the reader may consult the books by Zemanian (1965, 1968). Lavoine (1963) contains tables of Fourier transforms of distributions.

1.3.2.5.2. $\mathscr{S}$ *as a test-function space*

A notion of convergence has to be introduced in $\mathscr{S}(\mathbb{R}^n)$ in order to be able to define and test the continuity of linear functionals on it.

A sequence (φ_j) of functions in $\mathscr{S}$ will be said to converge to 0 if, for any given multi-indices $\mathbf{k}$ and $\mathbf{p}$, the sequence $(\mathbf{x}^{\mathbf{k}}D^{\mathbf{p}}\varphi_j)$ tends to 0 uniformly on $\mathbb{R}^n$.

It can be shown that $\mathscr{D}(\mathbb{R}^n)$ is dense in $\mathscr{S}(\mathbb{R}^n)$. Translation is continuous for this topology. For any linear differential operator $P(D) = \sum_{\mathbf{p}} a_{\mathbf{p}} D^{\mathbf{p}}$ and any polynomial $Q(\mathbf{x})$ over $\mathbb{R}^n$, $(\varphi_j) \to 0$ implies $[Q(\mathbf{x}) \times P(D)\varphi_j] \to 0$ in the topology of $\mathscr{S}$. Therefore, differentiation and multiplication by polynomials are continuous for the topology on $\mathscr{S}$.

The Fourier transformations $\mathscr{F}$ and $\bar{\mathscr{F}}$ are also continuous for the topology of $\mathscr{S}$. Indeed, let (φ_j) converge to 0 for the topology on $\mathscr{S}$. Then, by Section 1.3.2.4.2,

$$\|(2\pi\boldsymbol{\xi})^{\mathbf{m}} D^{\mathbf{p}}(\mathscr{F}[\varphi_j])\|_\infty \leq \|D^{\mathbf{m}}[(2\pi\mathbf{x})^{\mathbf{p}}\varphi_j]\|_1.$$

The right-hand side tends to 0 as $j \to \infty$ by definition of convergence in $\mathscr{S}$, hence $\|\boldsymbol{\xi}\|^{\mathbf{m}} D^{\mathbf{p}}(\mathscr{F}[\varphi_j]) \to 0$ uniformly, so that $(\mathscr{F}[\varphi_j]) \to 0$ in $\mathscr{S}$ as $j \to \infty$. The same proof applies to $\bar{\mathscr{F}}$.

1.3.2.5.3. *Definition and examples of tempered distributions*

A distribution $T \in \mathscr{D}'(\mathbb{R}^n)$ is said to be *tempered* if it can be extended into a continuous linear functional on $\mathscr{S}$.

If $\mathscr{S}'(\mathbb{R}^n)$ is the topological dual of $\mathscr{S}(\mathbb{R}^n)$, and if $S \in \mathscr{S}'(\mathbb{R}^n)$, then its restriction to $\mathscr{D}$ is a tempered distribution; conversely, if $T \in \mathscr{D}'$ is tempered, then its extension to $\mathscr{S}$ is unique (because $\mathscr{D}$ is dense in $\mathscr{S}$), hence it defines an element S of $\mathscr{S}'$. We may therefore identify $\mathscr{S}'$ and the space of tempered distributions.

A distribution with compact support is tempered, *i.e.* $\mathscr{S}' \supset \mathscr{E}'$. By transposition of the corresponding properties of $\mathscr{S}$, it is readily established that the derivative, translate or product by a polynomial of a tempered distribution is still a tempered distribution.

These inclusion relations may be summarized as follows: since $\mathscr{S}$ contains $\mathscr{D}$ but is contained in $\mathscr{E}$, the reverse inclusions hold for the topological duals, and hence $\mathscr{S}'$ contains $\mathscr{E}'$ but is contained in $\mathscr{D}'$.

A locally summable function f on $\mathbb{R}^n$ will be said to be *of polynomial growth* if $|f(\mathbf{x})|$ can be majorized by a polynomial in $\|\mathbf{x}\|$ as $\|\mathbf{x}\| \to \infty$. It is easily shown that such a function f defines a tempered distribution T_f *via*

$$\langle T_f, \varphi\rangle = \int_{\mathbb{R}^n} f(\mathbf{x})\varphi(\mathbf{x})\, \mathrm{d}^n\mathbf{x}.$$

In particular, polynomials over $\mathbb{R}^n$ define tempered distributions, and so do functions in $\mathscr{S}$. The latter remark, together with the transposition identity (Section 1.3.2.4.4), invites the extension of $\mathscr{F}$ and $\bar{\mathscr{F}}$ from $\mathscr{S}$ to $\mathscr{S}'$.

1.3.2.5.4. *Fourier transforms of tempered distributions*

The Fourier transform $\mathscr{F}[T]$ and cotransform $\bar{\mathscr{F}}[T]$ of a tempered distribution T are defined by

$$\langle \mathscr{F}[T], \varphi\rangle = \langle T, \mathscr{F}[\varphi]\rangle$$
$$\langle \bar{\mathscr{F}}[T], \varphi\rangle = \langle T, \bar{\mathscr{F}}[\varphi]\rangle$$

for all test functions $\varphi \in \mathscr{S}$. Both $\mathscr{F}[T]$ and $\bar{\mathscr{F}}[T]$ are themselves tempered distributions, since the maps $\varphi \longmapsto \mathscr{F}[\varphi]$ and $\varphi \longmapsto \bar{\mathscr{F}}[\varphi]$ are both linear and continuous for the topology of $\mathscr{S}$. In the same way that $\mathbf{x}$ and $\boldsymbol{\xi}$ have been used consistently as arguments for φ and $\mathscr{F}[\varphi]$, respectively, the notation $T_{\mathbf{x}}$ and $\mathscr{F}[T]_{\boldsymbol{\xi}}$ will be used to indicate which variables are involved.

When T is a distribution with compact support, its Fourier transform may be written

$$\mathscr{F}[T_{\mathbf{x}}]_{\boldsymbol{\xi}} = \langle T_{\mathbf{x}}, \exp(-2\pi i\boldsymbol{\xi}\cdot\mathbf{x})\rangle$$

since the function $\mathbf{x} \longmapsto \exp(-2\pi i\boldsymbol{\xi}\cdot\mathbf{x})$ is in $\mathscr{E}$ while $T_{\mathbf{x}} \in \mathscr{E}'$. It can be shown, as in Section 1.3.2.4.2, to be analytically continuable into an entire function over $\mathbb{C}^n$.

1.3.2.5.5. *Transposition of basic properties*

The duality between differentiation and multiplication by a monomial extends from $\mathscr{S}$ to $\mathscr{S}'$ by transposition:

$$\mathscr{F}[D_{\mathbf{x}}^{\mathbf{p}} T_{\mathbf{x}}]_{\boldsymbol{\xi}} = (2\pi i\boldsymbol{\xi})^{\mathbf{p}} \mathscr{F}[T_{\mathbf{x}}]_{\boldsymbol{\xi}}$$
$$D_{\boldsymbol{\xi}}^{\mathbf{p}}(\mathscr{F}[T_{\mathbf{x}}]_{\boldsymbol{\xi}}) = \mathscr{F}[(-2\pi i\mathbf{x})^{\mathbf{p}} T_{\mathbf{x}}]_{\boldsymbol{\xi}}.$$

Analogous formulae hold for $\bar{\mathscr{F}}$, with i replaced by $-i$.

The formulae expressing the duality between translation and phase shift, *e.g.*

$$\mathscr{F}[\tau_{\mathbf{a}} T_{\mathbf{x}}]_{\boldsymbol{\xi}} = \exp(-2\pi i\mathbf{a}\cdot\boldsymbol{\xi})\mathscr{F}[T_{\mathbf{x}}]_{\boldsymbol{\xi}}$$
$$\tau_{\boldsymbol{\alpha}}(\mathscr{F}[T_{\mathbf{x}}]_{\boldsymbol{\xi}}) = \mathscr{F}[\exp(2\pi i\boldsymbol{\alpha}\cdot\mathbf{x})T_{\mathbf{x}}]_{\boldsymbol{\xi}};$$

between a linear change of variable and its contragredient, *e.g.*

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

are obtained similarly by transposition from the corresponding identities in $\mathscr{S}$. They give a transposition formula for an affine change of variables $\mathbf{x} \longmapsto S(\mathbf{x}) = \mathbf{A}\mathbf{x} + \mathbf{b}$ with non-singular matrix $\mathbf{A}$:

$$\begin{aligned}\mathscr{F}[S^{\#}T] &= \exp(-2\pi i\boldsymbol{\xi}\cdot\mathbf{b})\mathscr{F}[A^{\#}T] \\ &= \exp(-2\pi i\boldsymbol{\xi}\cdot\mathbf{b})|\det \mathbf{A}|[(\mathbf{A}^{-1})^T]^{\#}\mathscr{F}[T],\end{aligned}$$

with a similar result for $\bar{\mathscr{F}}$, replacing $-i$ by $+i$.

Conjugate symmetry is obtained similarly:

$$\mathscr{F}[\bar{T}] = \breve{\overline{\mathscr{F}[T]}}, \mathscr{F}[\breve{\bar{T}}] = \overline{\mathscr{F}[T]},$$

with the same identities for $\bar{\mathscr{F}}$.

The tensor product property also transposes to tempered distributions: if $U \in \mathscr{S}'(\mathbb{R}^m)$, $V \in \mathscr{S}'(\mathbb{R}^n)$,

$$\mathscr{F}[U_{\mathbf{x}} \otimes V_{\mathbf{y}}] = \mathscr{F}[U]_{\boldsymbol{\xi}} \otimes \mathscr{F}[V]_{\boldsymbol{\eta}}$$
$$\bar{\mathscr{F}}[U_{\mathbf{x}} \otimes V_{\mathbf{y}}] = \bar{\mathscr{F}}[U]_{\boldsymbol{\xi}} \otimes \bar{\mathscr{F}}[V]_{\boldsymbol{\eta}}.$$

1.3.2.5.6. *Transforms of* δ*-functions*

Since δ has compact support,

$$\mathscr{F}[\delta_{\mathbf{x}}]_{\boldsymbol{\xi}} = \langle \delta_{\mathbf{x}}, \exp(-2\pi i\boldsymbol{\xi}\cdot\mathbf{x})\rangle = 1_{\boldsymbol{\xi}}, \quad \textit{i.e. } \mathscr{F}[\delta] = 1.$$

It is instructive to show that conversely $\mathscr{F}[1] = \delta$ without invoking the reciprocity theorem. Since $\partial_j 1 = 0$ for all $j = 1, \ldots, n$, it follows from Section 1.3.2.3.9.4 that $\mathscr{F}[1] = c\delta$; the constant c can be determined by using the invariance of the standard Gaussian G established in Section 1.3.2.4.3:

$$\langle \mathscr{F}[1]_{\mathbf{x}}, G_{\mathbf{x}}\rangle = \langle 1_{\boldsymbol{\xi}}, G_{\boldsymbol{\xi}}\rangle = 1;$$

hence $c = 1$. Thus, $\mathscr{F}[1] = \delta$.

The basic properties above then read (using multi-indices to denote differentiation):

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

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-*