International Tables for Crystallography (2006). Vol. B, Section 1.3.2.3.9.7, pp. 33–34.

1.3.2.3.9.4. *Division of distributions by functions*

Given a distribution S on $\mathbb{R}^n$ and an infinitely differentiable multiplier function α, the division problem consists in finding a distribution T such that $\alpha T = S$.

If α never vanishes, $T = S/\alpha$ is the unique answer. If $n = 1$, and if α has only isolated zeros of finite order, it can be reduced to a collection of cases where the multiplier is x^m, for which the general solution can be shown to be of the form

$$T = U + \sum_{i=0}^{m-1} c_i \delta^{(i)},$$

where U is a particular solution of the division problem $x^m U = S$ and the c_i are arbitrary constants.

In dimension $n > 1$, the problem is much more difficult, but is of fundamental importance in the theory of linear partial differential equations, since the Fourier transformation turns the problem of solving these into a division problem for distributions [see Hörmander (1963)].

1.3.2.3.9.5. *Transformation of coordinates*

Let σ be a smooth non-singular change of variables in $\mathbb{R}^n$, *i.e.* an infinitely differentiable mapping from an open subset Ω of $\mathbb{R}^n$ to Ω' in $\mathbb{R}^n$, whose Jacobian

$$J(\sigma) = \det \left[\frac{\partial \sigma(\mathbf{x})}{\partial \mathbf{x}}\right]$$

vanishes nowhere in Ω. By the implicit function theorem, the inverse mapping σ^{-1} from Ω' to Ω is well defined.

If f is a locally summable function on Ω, then the function $\sigma^{\#} f$ defined by

$$(\sigma^{\#} f)(\mathbf{x}) = f[\sigma^{-1}(\mathbf{x})]$$

is a locally summable function on Ω', and for any $\varphi \in \mathcal{D}(\Omega')$ we may write:

$$\begin{aligned}\int_{\Omega'} (\sigma^{\#} f)(\mathbf{x})\varphi(\mathbf{x}) \,\mathrm{d}^n\mathbf{x} &= \int_{\Omega'} f[\sigma^{-1}(\mathbf{x})]\varphi(\mathbf{x}) \,\mathrm{d}^n\mathbf{x}\\ &= \int_{\Omega'} f(\mathbf{y})\varphi[\sigma(\mathbf{y})]|J(\sigma)| \,\mathrm{d}^n\mathbf{y} \quad \text{by } \mathbf{x} = \sigma(\mathbf{y}).\end{aligned}$$

In terms of the associated distributions

$$\langle T_{\sigma^{\#} f}, \varphi\rangle = \langle T_f, |J(\sigma)|(\sigma^{-1})^{\#}\varphi\rangle.$$

This operation can be extended to an arbitrary distribution T by defining its *image* $\sigma^{\#} T$ under coordinate transformation σ through

$$\langle \sigma^{\#} T, \varphi\rangle = \langle T, |J(\sigma)|(\sigma^{-1})^{\#}\varphi\rangle,$$

which is well defined provided that σ is *proper*, *i.e.* that $\sigma^{-1}(K)$ is compact whenever K is compact.

For instance, if $\sigma : \mathbf{x} \longmapsto \mathbf{x} + \mathbf{a}$ is a *translation* by a vector $\mathbf{a}$ in $\mathbb{R}^n$, then $|J(\sigma)| = 1$; $\sigma^{\#}$ is denoted by $\tau_{\mathbf{a}}$, and the translate $\tau_{\mathbf{a}} T$ of a distribution T is defined by

$$\langle \tau_{\mathbf{a}} T, \varphi\rangle = \langle T, \tau_{-\mathbf{a}}\varphi\rangle.$$

Let $A : \mathbf{x} \longmapsto \mathbf{A}\mathbf{x}$ be a linear transformation defined by a non-singular matrix $\mathbf{A}$. Then $J(A) = \det \mathbf{A}$, and

$$\langle A^{\#} T, \varphi\rangle = |\det \mathbf{A}|\langle T, (A^{-1})^{\#}\varphi\rangle.$$

This formula will be shown later (Sections 1.3.2.6.5, 1.3.4.2.1.1) to be the basis for the definition of the reciprocal lattice.

In particular, if $\mathbf{A} = -\mathbf{I}$, where $\mathbf{I}$ is the identity matrix, A is an inversion through a centre of symmetry at the origin, and denoting $A^{\#}\varphi$ by $\breve{\varphi}$ we have:

$$\langle \breve{T}, \varphi\rangle = \langle T, \breve{\varphi}\rangle.$$

T is called an even distribution if $\breve{T} = T$, an odd distribution if $\breve{T} = -T$.

If $\mathbf{A} = \lambda \mathbf{I}$ with $\lambda > 0$, A is called a *dilation* and

$$\langle A^{\#} T, \varphi\rangle = \lambda^n \langle T, (A^{-1})^{\#}\varphi\rangle.$$

Writing symbolically δ as $\delta(\mathbf{x})$ and $A^{\#}\delta$ as $\delta(\mathbf{x}/\lambda)$, we have:

$$\delta(\mathbf{x}/\lambda) = \lambda^n \delta(\mathbf{x}).$$

If $n = 1$ and f is a function with isolated simple zeros x_j, then in the same symbolic notation

$$\delta[f(x)] = \sum_j \frac{1}{|f'(x_j)|}\delta(x_j),$$

where each $\lambda_j = 1/|f'(x_j)|$ is analogous to a 'Lorentz factor' at zero x_j.

1.3.2.3.9.6. *Tensor product of distributions*

The purpose of this construction is to extend Fubini's theorem to distributions. Following Section 1.3.2.2.5, we may define the tensor product $L^1_{\text{loc}}(\mathbb{R}^m) \otimes L^1_{\text{loc}}(\mathbb{R}^n)$ as the vector space of finite linear combinations of functions of the form

$$f \otimes g : (\mathbf{x}, \mathbf{y}) \longmapsto f(\mathbf{x})g(\mathbf{y}),$$

where $\mathbf{x} \in \mathbb{R}^m$, $\mathbf{y} \in \mathbb{R}^n$, $f \in L^1_{\text{loc}}(\mathbb{R}^m)$ and $g \in L^1_{\text{loc}}(\mathbb{R}^n)$.

Let $S_{\mathbf{x}}$ and $T_{\mathbf{y}}$ denote the distributions associated to f and g, respectively, the subscripts $\mathbf{x}$ and $\mathbf{y}$ acting as mnemonics for $\mathbb{R}^m$ and $\mathbb{R}^n$. It follows from Fubini's theorem (Section 1.3.2.2.5) that $f \otimes g \in L^1_{\text{loc}}(\mathbb{R}^m \times \mathbb{R}^n)$, and hence defines a distribution over $\mathbb{R}^m \times \mathbb{R}^n$; the rearrangement of integral signs gives

$$\langle S_{\mathbf{x}} \otimes T_{\mathbf{y}}, \varphi_{\mathbf{x},\mathbf{y}}\rangle = \langle S_{\mathbf{x}}, \langle T_{\mathbf{y}}, \varphi_{\mathbf{x},\mathbf{y}}\rangle\rangle = \langle T_{\mathbf{y}}, \langle S_{\mathbf{x}}, \varphi_{\mathbf{x},\mathbf{y}}\rangle\rangle$$

for all $\varphi_{\mathbf{x},\mathbf{y}} \in \mathcal{D}(\mathbb{R}^m \times \mathbb{R}^n)$. In particular, if $\varphi(\mathbf{x}, \mathbf{y}) = u(\mathbf{x})v(\mathbf{y})$ with $u \in \mathcal{D}(\mathbb{R}^m)$, $v \in \mathcal{D}(\mathbb{R}^n)$, then

$$\langle S \otimes T, u \otimes v\rangle = \langle S, u\rangle\langle T, v\rangle.$$

This construction can be extended to general distributions $S \in \mathcal{D}'(\mathbb{R}^m)$ and $T \in \mathcal{D}'(\mathbb{R}^n)$. Given any test function $\varphi \in \mathcal{D}(\mathbb{R}^m \times \mathbb{R}^n)$, let $\varphi_{\mathbf{x}}$ denote the map $\mathbf{y} \longmapsto \varphi(\mathbf{x}, \mathbf{y})$; let $\varphi_{\mathbf{y}}$ denote the map $\mathbf{x} \longmapsto \varphi(\mathbf{x}, \mathbf{y})$; and define the two functions $\theta(\mathbf{x}) = \langle T, \varphi_{\mathbf{x}}\rangle$ and $\omega(\mathbf{y}) = \langle S, \varphi_{\mathbf{y}}\rangle$. Then, by the lemma on differentiation under the $\langle,\rangle$ sign of Section 1.3.2.3.9.1, $\theta \in \mathcal{D}(\mathbb{R}^m)$, $\omega \in \mathcal{D}(\mathbb{R}^n)$, and there exists a unique distribution $S \otimes T$ such that

$$\langle S \otimes T, \varphi\rangle = \langle S, \theta\rangle = \langle T, \omega\rangle.$$

$S \otimes T$ is called the *tensor product* of S and T.

With the mnemonic introduced above, this definition reads identically to that given above for distributions associated to locally integrable functions:

$$\langle S_{\mathbf{x}} \otimes T_{\mathbf{y}}, \varphi_{\mathbf{x},\mathbf{y}}\rangle = \langle S_{\mathbf{x}}, \langle T_{\mathbf{y}}, \varphi_{\mathbf{x},\mathbf{y}}\rangle\rangle = \langle T_{\mathbf{y}}, \langle S_{\mathbf{x}}, \varphi_{\mathbf{x},\mathbf{y}}\rangle\rangle.$$

The tensor product of distributions is associative:

$$(R \otimes S) \otimes T = R \otimes (S \otimes T).$$

Derivatives may be calculated by

$$D^{\mathbf{p}}_{\mathbf{x}} D^{\mathbf{q}}_{\mathbf{y}} (S_{\mathbf{x}} \otimes T_{\mathbf{y}}) = (D^{\mathbf{p}}_{\mathbf{x}} S_{\mathbf{x}}) \otimes (D^{\mathbf{q}}_{\mathbf{y}} T_{\mathbf{y}}).$$

The support of a tensor product is the Cartesian product of the supports of the two factors.

1.3.2.3.9.7. *Convolution of distributions*

The convolution $f * g$ of two functions f and g on $\mathbb{R}^n$ is defined by

$$(f * g)(\mathbf{x}) = \int_{\mathbb{R}^n} f(\mathbf{y})g(\mathbf{x} - \mathbf{y}) \,\mathrm{d}^n\mathbf{y} = \int_{\mathbb{R}^n} f(\mathbf{x} - \mathbf{y})g(\mathbf{y}) \,\mathrm{d}^n\mathbf{y}$$

whenever the integral exists. This is the case when f and g are both in $L^1(\mathbb{R}^n)$; then $f * g$ is also in $L^1(\mathbb{R}^n)$. Let S, T and W denote the distributions associated to f, g and $f * g$, respectively: a change of variable immediately shows that for any $\varphi \in \mathcal{D}(\mathbb{R}^n)$,

$$\langle W, \varphi \rangle = \int\limits_{\mathbb{R}^n \times \mathbb{R}^n} f(\mathbf{x}) g(\mathbf{y}) \varphi(\mathbf{x} + \mathbf{y}) \, \mathrm{d}^n\mathbf{x} \, \mathrm{d}^n\mathbf{y}.$$

Introducing the map σ from $\mathbb{R}^n \times \mathbb{R}^n$ to $\mathbb{R}^n$ defined by $\sigma(\mathbf{x}, \mathbf{y}) = \mathbf{x} + \mathbf{y}$, the latter expression may be written:

$$\langle S_{\mathbf{x}} \otimes T_{\mathbf{y}}, \varphi \circ \sigma \rangle$$

(where $\circ$ denotes the composition of mappings) or by a slight abuse of notation:

$$\langle W, \varphi \rangle = \langle S_{\mathbf{x}} \otimes T_{\mathbf{y}}, \varphi(\mathbf{x} + \mathbf{y}) \rangle.$$

A difficulty arises in extending this definition to general distributions S and T because the mapping σ is not proper: if K is compact in $\mathbb{R}^n$, then $\sigma^{-1}(K)$ is a cylinder with base K and generator the 'second bisector' $\mathbf{x} + \mathbf{y} = \mathbf{0}$ in $\mathbb{R}^n \times \mathbb{R}^n$. However, $\langle S \otimes T, \varphi \circ \sigma \rangle$ is defined whenever the intersection between Supp $(S \otimes T) =$ (Supp S) $\times$ (Supp T) and σ^{-1}(Supp φ) is compact.

We may therefore define the *convolution* $S * T$ of two distributions S and T on $\mathbb{R}^n$ by

$$\langle S * T, \varphi \rangle = \langle S \otimes T, \varphi \circ \sigma \rangle = \langle S_{\mathbf{x}} \otimes T_{\mathbf{y}}, \varphi(\mathbf{x} + \mathbf{y}) \rangle$$

whenever the following *support condition* is fulfilled:

'the set $\{(\mathbf{x}, \mathbf{y}) | \mathbf{x} \in A, \mathbf{y} \in B, \mathbf{x} + \mathbf{y} \in K\}$ is compact in $\mathbb{R}^n \times \mathbb{R}^n$ for all K compact in $\mathbb{R}^n$'.

The latter condition is met, in particular, if S or T has compact support. The support of $S * T$ is easily seen to be contained in the closure of the vector sum

$$A + B = \{\mathbf{x} + \mathbf{y} | \mathbf{x} \in A, \mathbf{y} \in B\}.$$

Convolution by a fixed distribution S is a *continuous* operation for the topology on $\mathcal{D}'$: it maps convergent sequences (T_j) to convergent sequences $(S * T_j)$. Convolution is commutative: $S * T = T * S$.

The convolution of p distributions $T_1, \ldots, T_p$ with supports $A_1, \ldots, A_p$ can be defined by

$$\langle T_1 * \ldots * T_p, \varphi \rangle = \langle (T_1)_{\mathbf{x}_1} \otimes \ldots \otimes (T_p)_{\mathbf{x}_p}, \varphi(\mathbf{x}_1 + \ldots + \mathbf{x}_p) \rangle$$

whenever the following generalized support condition:

'the set $\{(\mathbf{x}_1, \ldots, \mathbf{x}_p) | \mathbf{x}_1 \in A_1, \ldots, \mathbf{x}_p \in A_p, \mathbf{x}_1 + \ldots + \mathbf{x}_p \in K\}$ is compact in $(\mathbb{R}^n)^p$ for all K compact in $\mathbb{R}^n$'

is satisfied. It is then associative. Interesting examples of associativity failure, which can be traced back to violations of the support condition, may be found in Bracewell (1986, pp. 436–437).

It follows from previous definitions that, for all distributions $T \in \mathcal{D}'$, the following identities hold:

(i) $\delta * T = T$: δ is the unit convolution;

(ii) $\delta_{(\mathbf{a})} * T = \tau_{\mathbf{a}} T$: translation is a convolution with the corresponding translate of δ;

(iii) $(D^{\mathbf{p}} \delta) * T = D^{\mathbf{p}} T$: differentiation is a convolution with the corresponding derivative of δ;

(iv) translates or derivatives of a convolution may be obtained by translating or differentiating any one of the factors: convolution 'commutes' with translation and differentiation, a property used in Section 1.3.4.4.7.7 to speed up least-squares model refinement for macromolecules.

The latter property is frequently used for the purpose of *regularization*: if T is a distribution, α an infinitely differentiable function, and at least one of the two has compact support, then $T * \alpha$ is an infinitely differentiable ordinary function. Since sequences (α_ν) of such functions α can be constructed which have compact support and converge to δ, it follows that any distribution T can be obtained as the limit of infinitely differentiable functions $T * \alpha_\nu$. In topological jargon: $\mathcal{D}(\mathbb{R}^n)$ is 'everywhere dense' in $\mathcal{D}'(\mathbb{R}^n)$. A standard function in $\mathcal{D}$ which is often used for such proofs is defined as follows: put

$$\begin{aligned} \theta(x) &= \frac{1}{A} \exp\left(-\frac{1}{1 - x^2}\right) \quad \text{for } |x| \leq 1, \\ &= 0 \qquad\qquad\qquad\qquad \text{for } |x| \geq 1, \end{aligned}$$

with

$$A = \int\limits_{-1}^{+1} \exp\left(-\frac{1}{1 - x^2}\right) \mathrm{d}x$$

(so that θ is in $\mathcal{D}$ and is normalized), and put

$$\begin{aligned} \theta_\varepsilon(x) &= \frac{1}{\varepsilon} \theta\left(\frac{x}{\varepsilon}\right) \quad \text{in dimension 1,} \\ \theta_\varepsilon(\mathbf{x}) &= \prod_{j=1}^{n} \theta_\varepsilon(x_j) \quad \text{in dimension } n. \end{aligned}$$

Another related result, also proved by convolution, is the *structure theorem*: the restriction of a distribution $T \in \mathcal{D}'(\mathbb{R}^n)$ to a bounded open set Ω in $\mathbb{R}^n$ is a derivative of finite order of a continuous function.

Properties (i) to (iv) are the basis of the symbolic or operational calculus (see Carslaw & Jaeger, 1948; Van der Pol & Bremmer, 1955; Churchill, 1958; Erdélyi, 1962; Moore, 1971) for solving integro-differential equations with constant coefficients by turning them into convolution equations, then using factorization methods for convolution algebras (Schwartz, 1965).

1.3.2.4. *Fourier transforms of functions*

1.3.2.4.1. *Introduction*

Given a complex-valued function f on $\mathbb{R}^n$ subject to suitable regularity conditions, its Fourier transform $\mathcal{F}[f]$ and Fourier cotransform $\bar{\mathcal{F}}[f]$ are defined as follows:

$$\begin{aligned} \mathcal{F}[f](\xi) &= \int\limits_{\mathbb{R}^n} f(\mathbf{x}) \exp(-2\pi i \boldsymbol{\xi} \cdot \mathbf{x}) \, \mathrm{d}^n\mathbf{x} \\ \bar{\mathcal{F}}[f](\xi) &= \int\limits_{\mathbb{R}^n} f(\mathbf{x}) \exp(+2\pi i \boldsymbol{\xi} \cdot \mathbf{x}) \, \mathrm{d}^n\mathbf{x}, \end{aligned}$$

where $\boldsymbol{\xi} \cdot \mathbf{x} = \sum_{i=1}^{n} \xi_i x_i$ is the ordinary scalar product. The terminology and sign conventions given above are the standard ones in mathematics; those used in crystallography are slightly different (see Section 1.3.4.2.1.1). These transforms enjoy a number of remarkable properties, whose natural settings entail different regularity assumptions on f: for instance, properties relating to convolution are best treated in $L^1(\mathbb{R}^n)$, while Parseval's theorem requires the Hilbert space structure of $L^2(\mathbb{R}^n)$. After a brief review of these classical properties, the Fourier transformation will be examined in a space $\mathcal{S}(\mathbb{R}^n)$ particularly well suited to accommodating the full range of its properties, which will later serve as a space of test functions to extend the Fourier transformation to distributions.

There exists an abundant literature on the 'Fourier integral'. The books by Carslaw (1930), Wiener (1933), Titchmarsh (1948), Katznelson (1968), Sneddon (1951, 1972), and Dym & McKean (1972) are particularly recommended.

references