

1.3. FOURIER TRANSFORMS IN CRYSTALLOGRAPHY

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:

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

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 $\sigma: \mathbf{x} \mapsto \mathbf{x} + \mathbf{a}$ 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 $A: \mathbf{x} \mapsto \mathbf{A}\mathbf{x}$ 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 $\check{\varphi}$ we have:

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

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

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

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

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 $\mathbf{y} \mapsto \varphi(\mathbf{x}, \mathbf{y})$; let $\varphi_{\mathbf{y}}$ denote the map $\mathbf{x} \mapsto \varphi(\mathbf{x}, \mathbf{y})$; 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

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

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

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