

## 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  $\alpha$ , the division problem consists in finding a distribution  $T$  such that  $\alpha T = S$ .

If  $\alpha$  never vanishes,  $T = S/\alpha$  is the unique answer. If  $n = 1$ , and if  $\alpha$  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  $\sigma$  be a smooth non-singular change of variables in  $\mathbb{R}^n$ , i.e. an infinitely differentiable mapping from an open subset  $\Omega$  of  $\mathbb{R}^n$  to  $\Omega'$  in  $\mathbb{R}^n$ , whose Jacobian

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

vanishes nowhere in  $\Omega$ . By the implicit function theorem, the inverse mapping  $\sigma^{-1}$  from  $\Omega'$  to  $\Omega$  is well defined.

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

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

is a locally summable function on  $\Omega'$ , 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  $\sigma$  through

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

which is well defined provided that  $\sigma$  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  $\delta$  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  $L_{\text{loc}}^1(\mathbb{R}^m) \otimes L_{\text{loc}}^1(\mathbb{R}^n)$  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  $\mathbf{x} \in \mathbb{R}^m, \mathbf{y} \in \mathbb{R}^n, f \in L_{\text{loc}}^1(\mathbb{R}^m)$  and  $g \in L_{\text{loc}}^1(\mathbb{R}^n)$ .

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  $f \otimes g \in L_{\text{loc}}^1(\mathbb{R}^m \times \mathbb{R}^n)$ , 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

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