International Tables for Crystallography (2010). Vol. B, Section 1.3.2.3.9.4, pp. 32–33.

Let f be infinitely differentiable for $x < 0$ and $x > 0$ but have discontinuous derivatives $f^{(m)}$ at $x = 0$ [$f^{(0)}$ being f itself] with jumps $\sigma_m = f^{(m)}(0+) - f^{(m)}(0-)$. Consider the functions:

$$\begin{aligned} g_0 &= f - \sigma_0 Y \\ g_1 &= g_0' - \sigma_1 Y \\ &\text{-----------} \\ g_k &= g_{k-1}' - \sigma_k Y. \end{aligned}$$

The g_k are continuous, their derivatives g_k' are continuous almost everywhere [which implies that $(T_{g_k})' = T_{g_k'}$ and $g_k' = f^{(k+1)}$ almost everywhere]. This yields immediately:

$$\begin{aligned} (T_f)' &= T_{f'} + \sigma_0 \delta \\ (T_f)'' &= T_{f''} + \sigma_0 \delta' + \sigma_1 \delta \\ &\text{-------------------} \\ (T_f)^{(m)} &= T_{f^{(m)}} + \sigma_0 \delta^{(m-1)} + \ldots + \sigma_{m-1}\delta. \\ &\text{-------------------} \end{aligned}$$

Thus the 'distributional derivatives' $(T_f)^{(m)}$ differ from the usual functional derivatives $T_{f^{(m)}}$ by singular terms associated with discontinuities.

In dimension n, let f be infinitely differentiable everywhere except on a smooth hypersurface S, across which its partial derivatives show discontinuities. Let σ_0 and σ_ν denote the discontinuities of f and its normal derivative $\partial_\nu \varphi$ across S (both σ_0 and σ_ν are functions of position on S), and let $\delta_{(S)}$ and $\partial_\nu \delta_{(S)}$ be defined by

$$\begin{aligned} \langle \delta_{(S)}, \varphi \rangle &= \int_S \varphi \, \mathrm{d}^{n-1} S \\ \langle \partial_\nu \delta_{(S)}, \varphi \rangle &= -\int_S \partial_\nu \varphi \, \mathrm{d}^{n-1} S. \end{aligned}$$

Integration by parts shows that

$$\partial_i T_f = T_{\partial_i f} + \sigma_0 \cos \theta_i \delta_{(S)},$$

where θ_i is the angle between the x_i axis and the normal to S along which the jump σ_0 occurs, and that the Laplacian of T_f is given by

$$\Delta(T_f) = T_{\Delta f} + \sigma_\nu \delta_{(S)} + \partial_\nu [\sigma_0 \delta_{(S)}].$$

The latter result is a statement of Green's theorem in terms of distributions. It will be used in Section 1.3.4.4.3.5 to calculate the Fourier transform of the indicator function of a molecular envelope.

1.3.2.3.9.2. Integration of distributions in dimension 1

The reverse operation from differentiation, namely calculating the 'indefinite integral' of a distribution S, consists in finding a distribution T such that $T' = S$.

For all $\chi \in \mathcal{D}$ such that $\chi = \psi'$ with $\psi \in \mathcal{D}$, we must have

$$\langle T, \chi \rangle = -\langle S, \psi \rangle.$$

This condition defines T in a 'hyperplane' $\mathcal{H}$ of $\mathcal{D}$, whose equation

$$\langle 1, \chi \rangle \equiv \langle 1, \psi' \rangle = 0$$

reflects the fact that ψ has compact support.

To specify T in the whole of $\mathcal{D}$, it suffices to specify the value of $\langle T, \varphi_0 \rangle$ where $\varphi_0 \in \mathcal{D}$ is such that $\langle 1, \varphi_0 \rangle = 1$: then any $\varphi \in \mathcal{D}$ may be written uniquely as

$$\varphi = \lambda \varphi_0 + \psi'$$

with

$$\lambda = \langle 1, \varphi \rangle, \qquad \chi = \varphi - \lambda \varphi_0, \qquad \psi(x) = \int_0^x \chi(t) \, \mathrm{d}t,$$

and T is defined by

$$\langle T, \varphi \rangle = \lambda \langle T, \varphi_0 \rangle - \langle S, \psi \rangle.$$

The freedom in the choice of φ_0 means that T is defined up to an additive constant.

1.3.2.3.9.3. Multiplication of distributions by functions

The product αT of a distribution T on $\mathbb{R}^n$ by a function α over $\mathbb{R}^n$ will be defined by transposition:

$$\langle \alpha T, \varphi \rangle = \langle T, \alpha \varphi \rangle \quad \text{for all } \varphi \in \mathcal{D}.$$

In order that αT be a distribution, the mapping $\varphi \longmapsto \alpha \varphi$ must send $\mathcal{D}(\mathbb{R}^n)$ continuously into itself; hence *the multipliers* α *must be infinitely differentiable*. The product of two general distributions cannot be defined. The need for a careful treatment of multipliers of distributions will become clear when it is later shown (Section 1.3.2.5.8) that the Fourier transformation turns convolutions into multiplications and *vice versa*.

If T is a distribution of order m, then α needs only have continuous derivatives up to order m. For instance, δ is a distribution of order zero, and $\alpha\delta = \alpha(\mathbf{0})\delta$ is a distribution provided α is continuous; this relation is of fundamental importance in the theory of sampling and of the properties of the Fourier transformation related to sampling (Sections 1.3.2.6.4, 1.3.2.6.6). More generally, $D^{\mathbf{p}}\delta$ is a distribution of order $|\mathbf{p}|$, and the following formula holds for all $\alpha \in \mathcal{D}^{(m)}$ with $m = |\mathbf{p}|$:

$$\alpha(D^{\mathbf{p}}\delta) = \sum_{\mathbf{q} \le \mathbf{p}} (-1)^{|\mathbf{p}-\mathbf{q}|} \binom{\mathbf{p}}{\mathbf{q}} (D^{\mathbf{p}-\mathbf{q}}\alpha)(\mathbf{0}) D^{\mathbf{q}}\delta.$$

The derivative of a product is easily shown to be

$$\partial_i(\alpha T) = (\partial_i \alpha) T + \alpha(\partial_i T)$$

and generally for any multi-index $\mathbf{p}$

$$D^{\mathbf{p}}(\alpha T) = \sum_{\mathbf{q} \le \mathbf{p}} \binom{\mathbf{p}}{\mathbf{q}} (D^{\mathbf{p}-\mathbf{q}}\alpha)(\mathbf{0}) D^{\mathbf{q}} T.$$

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 nonsingular 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 $\varphi \in \mathscr{D}(\Omega')$ 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 nonsingular 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 $\varphi_{\mathbf{x},\mathbf{y}} \in \mathscr{D}(\mathbb{R}^m \times \mathbb{R}^n)$. In particular, if $\varphi(\mathbf{x}, \mathbf{y}) = u(\mathbf{x})v(\mathbf{y})$ with $u \in \mathscr{D}(\mathbb{R}^m)$, $v \in \mathscr{D}(\mathbb{R}^n)$, 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 $S \in \mathscr{D}'(\mathbb{R}^m)$ and $T \in \mathscr{D}'(\mathbb{R}^n)$. Given any test function $\varphi \in \mathscr{D}(\mathbb{R}^m \times \mathbb{R}^n)$, 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, $\theta \in \mathscr{D}(\mathbb{R}^m)$, $\omega \in \mathscr{D}(\mathbb{R}^n)$, and there exists a unique distribution $S \otimes T$ such that