International Tables for Crystallography (2006). Vol. B, Section 1.3.2.3.9.3, p. 32.

and let $\lambda_0 \in \Lambda$ be given parameter value. Suppose that, as λ runs through a small enough neighbourhood of λ_0,

(i) all the φ_λ have their supports in a fixed compact subset K of $\mathbb{R}^n$;

(ii) all the derivatives $D^{\mathbf{p}}\varphi_\lambda$ have a partial derivative with respect to λ which is continuous with respect to $\mathbf{x}$ and λ.

Under these hypotheses, $I(\lambda)$ is differentiable (in the usual sense) with respect to λ near λ_0, and its derivative may be obtained by 'differentiation under the $\langle,\rangle$ sign':

$$\frac{\mathrm{d}I}{\mathrm{d}\lambda} = \langle T, \partial_\lambda \varphi_\lambda \rangle.$$

(*c*) *Effect of discontinuities*

When a function *f* or its derivatives are no longer continuous, the derivatives $D^{\mathbf{p}}T_f$ of the associated distribution T_f may no longer coincide with the distributions associated to the functions $D^{\mathbf{p}}f$.

In dimension 1, the simplest example is Heaviside's unit step function Y [$Y(x) = 0$ for $x < 0, Y(x) = 1$ for $x \geq 0$]:

$$\langle (T_Y)', \varphi \rangle = -\langle (T_Y), \varphi' \rangle = -\int_0^{+\infty} \varphi'(x)\,\mathrm{d}x = \varphi(0) = \langle \delta, \varphi \rangle.$$

Hence $(T_Y)' = \delta$, a result long used 'heuristically' by electrical engineers [see also Dirac (1958)].

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:

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

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:

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

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

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

This condition defines *T* in a 'hyperplane' $\mathscr{H}$ of $\mathscr{D}$, 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 $\mathscr{D}$, it suffices to specify the value of $\langle T, \varphi_0 \rangle$ where $\varphi_0 \in \mathscr{D}$ is such that $\langle 1, \varphi_0 \rangle = 1$: then any $\varphi \in \mathscr{D}$ 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:

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

In order that αT be a distribution, the mapping $\varphi \longmapsto \alpha\varphi$ must send $\mathscr{D}(\mathbb{R}^n)$ 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 $\alpha \in \mathscr{D}^{(m)}$ with $m = |\mathbf{p}|$:

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

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 $\mathbf{p}$

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

references