

1.3. FOURIER TRANSFORMS IN CRYSTALLOGRAPHY

differential, partial differential and integral equations encountered in electrical engineering (today's 'signal processing'). These rules worked remarkably well but were devoid of mathematical justification (see Whittaker, 1928). In 1926, Dirac introduced his famous δ -function [see Dirac (1958), pp. 58–61], which was found to be related to Heaviside's constructs. Other singular objects, together with procedures to handle them, had already appeared in several branches of analysis [Cauchy's 'principal values'; Hadamard's 'finite parts' (Hadamard, 1932, 1952); Riesz's regularization methods for certain divergent integrals (Riesz, 1938, 1949)] as well as in the theories of Fourier series and integrals (see e.g. Bochner, 1932, 1959). Their very definition often verged on violating the rigorous rules governing limiting processes in analysis, so that subsequent recourse to limiting processes could lead to erroneous results; *ad hoc* precautions thus had to be observed to avoid mistakes in handling these objects.

In 1945–1950, Laurent Schwartz proposed his theory of distributions (see Schwartz, 1966), which provided a unified and definitive treatment of all these questions, with a striking combination of rigour and simplicity. Schwartz's treatment of Dirac's δ -function illustrates his approach in a most direct fashion. Dirac's original definition reads:

- (i) $\delta(\mathbf{x}) = 0$ for $\mathbf{x} \neq \mathbf{0}$,
- (ii) $\int_{\mathbb{R}^n} \delta(\mathbf{x}) d^n \mathbf{x} = 1$.

These two conditions are irreconcilable with Lebesgue's theory of integration: by (i), δ vanishes almost everywhere, so that its integral in (ii) must be 0, not 1.

A better definition consists in specifying that

$$(iii) \quad \int_{\mathbb{R}^n} \delta(\mathbf{x}) \varphi(\mathbf{x}) d^n \mathbf{x} = \varphi(\mathbf{0})$$

for any function φ sufficiently well behaved near $\mathbf{x} = \mathbf{0}$. This is related to the problem of finding a unit for convolution (Section 1.3.2.2.4). As will now be seen, this definition is still unsatisfactory. Let the sequence (f_ν) in $L^1(\mathbb{R}^n)$ be an approximate convolution unit, e.g.

$$f_\nu(\mathbf{x}) = \left(\frac{\nu}{2\pi} \right)^{1/2} \exp(-\frac{1}{2}\nu^2 \|\mathbf{x}\|^2).$$

Then for any well behaved function φ the integrals

$$\int_{\mathbb{R}^n} f_\nu(\mathbf{x}) \varphi(\mathbf{x}) d^n \mathbf{x}$$

exist, and the sequence of their numerical values tends to $\varphi(\mathbf{0})$. It is tempting to combine this with (iii) to conclude that δ is the limit of the sequence (f_ν) as $\nu \rightarrow \infty$. However,

$$\lim f_\nu(\mathbf{x}) = 0 \quad \text{as } \nu \rightarrow \infty$$

almost everywhere in \mathbb{R}^n and the crux of the problem is that

$$\begin{aligned} \varphi(\mathbf{0}) &= \lim_{\nu \rightarrow \infty} \int_{\mathbb{R}^n} f_\nu(\mathbf{x}) \varphi(\mathbf{x}) d^n \mathbf{x} \\ &\neq \int_{\mathbb{R}^n} \left[\lim_{\nu \rightarrow \infty} f_\nu(\mathbf{x}) \right] \varphi(\mathbf{x}) d^n \mathbf{x} = 0 \end{aligned}$$

because the sequence (f_ν) does not satisfy the hypotheses of Lebesgue's dominated convergence theorem.

Schwartz's solution to this problem is deceptively simple: the regular behaviour one is trying to capture is an attribute not of the sequence of functions (f_ν) , but of the sequence of continuous linear functionals

$$T_\nu : \varphi \mapsto \int_{\mathbb{R}^n} f_\nu(\mathbf{x}) \varphi(\mathbf{x}) d^n \mathbf{x}$$

which has as a limit the continuous functional

$$T : \varphi \mapsto \varphi(\mathbf{0}).$$

It is the latter functional which constitutes the proper definition of δ . The previous paradoxes arose because one insisted on writing down the simple linear operation T in terms of an integral.

The essence of Schwartz's theory of distributions is thus that, rather than try to define and handle 'generalized functions' via sequences such as (f_ν) [an approach adopted e.g. by Lighthill (1958) and Erdélyi (1962)], one should instead look at them as continuous linear functionals over spaces of well behaved functions.

There are many books on distribution theory and its applications. The reader may consult in particular Schwartz (1965, 1966), Gel'fand & Shilov (1964), Bremermann (1965), Trèves (1967), Challifour (1972), Friedlander (1982), and the relevant chapters of Hörmander (1963) and Yosida (1965). Schwartz (1965) is especially recommended as an introduction.

1.3.2.3.2. *Rationale*

The guiding principle which leads to requiring that the functions φ above (traditionally called 'test functions') should be well behaved is that correspondingly 'wilder' behaviour can then be accommodated in the limiting behaviour of the f_ν while still keeping the integrals $\int_{\mathbb{R}^n} f_\nu(\mathbf{x}) \varphi(\mathbf{x}) d^n \mathbf{x}$ under control. Thus

- (i) to minimize restrictions on the limiting behaviour of the f_ν at infinity, the φ 's will be chosen to have *compact support*;
- (ii) to minimize restrictions on the local behaviour of the f_ν , the φ 's will be chosen *infinitely differentiable*.

To ensure further the continuity of functionals such as T_ν with respect to the test function φ as the f_ν go increasingly wild, very strong control will have to be exercised in the way in which a sequence (φ_j) of test functions will be said to converge towards a limiting φ : conditions will have to be imposed not only on the values of the functions φ_j , but also on those of all their derivatives. Hence, defining a strong enough topology on the space of test functions φ is an essential prerequisite to the development of a satisfactory theory of distributions.

1.3.2.3.3. *Test-function spaces*

With this rationale in mind, the following function spaces will be defined for any open subset Ω of \mathbb{R}^n (which may be the whole of \mathbb{R}^n):

- (a) $\mathcal{E}(\Omega)$ is the space of complex-valued functions over Ω which are indefinitely differentiable;
- (b) $\mathcal{D}(\Omega)$ is the subspace of $\mathcal{E}(\Omega)$ consisting of functions with (unspecified) compact support contained in \mathbb{R}^n ;
- (c) $\mathcal{D}_K(\Omega)$ is the subspace of $\mathcal{D}(\Omega)$ consisting of functions whose (compact) support is contained within a fixed compact subset K of Ω .

When Ω is unambiguously defined by the context, we will simply write $\mathcal{E}, \mathcal{D}, \mathcal{D}_K$.

It sometimes suffices to require the existence of continuous derivatives only up to finite order m inclusive. The corresponding spaces are then denoted $\mathcal{E}^{(m)}, \mathcal{D}^{(m)}, \mathcal{D}_K^{(m)}$ with the convention that if $m = 0$, only continuity is required.

The topologies on these spaces constitute the most important ingredients of distribution theory, and will be outlined in some detail.

1.3.2.3.3.1. *Topology on $\mathcal{E}(\Omega)$*

It is defined by the family of semi-norms

$$\varphi \in \mathcal{E}(\Omega) \mapsto \sigma_{\mathbf{p}, K}(\varphi) = \sup_{\mathbf{x} \in K} |D^\mathbf{p} \varphi(\mathbf{x})|,$$

where \mathbf{p} is a multi-index and K a compact subset of Ω . A