

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

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

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,

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

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

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

which has as a limit the continuous functional

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

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

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

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

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fundamental system S of neighbourhoods of the origin in $\mathcal{E}(\Omega)$ is given by subsets of $\mathcal{E}(\Omega)$ of the form

$$V(m, \varepsilon, K) = \{\varphi \in \mathcal{E}(\Omega) \mid |\mathbf{p}| \leq m \Rightarrow \sigma_{\mathbf{p}, K}(\varphi) < \varepsilon\}$$

for all natural integers m , positive real ε , and compact subset K of Ω . Since a *countable* family of compact subsets K suffices to cover Ω , and since restricted values of ε of the form $\varepsilon = 1/N$ lead to the same topology, S is equivalent to a *countable* system of neighbourhoods and hence $\mathcal{E}(\Omega)$ is *metrizable*.

Convergence in \mathcal{E} may thus be defined by means of sequences. A sequence (φ_ν) in \mathcal{E} will be said to converge to 0 if for any given $V(m, \varepsilon, K)$ there exists ν_0 such that $\varphi_\nu \in V(m, \varepsilon, K)$ whenever $\nu > \nu_0$; in other words, if the φ_ν and all their derivatives $D^{\mathbf{p}}\varphi_\nu$ converge to 0 uniformly on any given compact K in Ω .

1.3.2.3.3.2. Topology on $\mathcal{Q}_K(\Omega)$

It is defined by the family of semi-norms

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

where K is now fixed. The fundamental system S of neighbourhoods of the origin in \mathcal{Q}_K is given by sets of the form

$$V(m, \varepsilon) = \{\varphi \in \mathcal{Q}_K(\Omega) \mid |\mathbf{p}| \leq m \Rightarrow \sigma_{\mathbf{p}}(\varphi) < \varepsilon\}.$$

It is equivalent to the countable subsystem of the $V(m, 1/N)$, hence $\mathcal{Q}_K(\Omega)$ is *metrizable*.

Convergence in \mathcal{Q}_K may thus be defined by means of sequences. A sequence (φ_ν) in \mathcal{Q}_K will be said to converge to 0 if for any given $V(m, \varepsilon)$ there exists ν_0 such that $\varphi_\nu \in V(m, \varepsilon)$ whenever $\nu > \nu_0$; in other words, if the φ_ν and all their derivatives $D^{\mathbf{p}}\varphi_\nu$ converge to 0 uniformly in K .

1.3.2.3.3.3. Topology on $\mathcal{Q}(\Omega)$

It is defined by the fundamental system of neighbourhoods of the origin consisting of sets of the form

$$V((m), (\varepsilon)) = \left\{ \varphi \in \mathcal{Q}(\Omega) \mid |\mathbf{p}| \leq m_\nu \Rightarrow \sup_{\|\mathbf{x}\| \leq \nu} |D^{\mathbf{p}}\varphi(\mathbf{x})| < \varepsilon_\nu \text{ for all } \nu \right\},$$

where (m) is an increasing sequence (m_ν) of integers tending to $+\infty$ and (ε) is a decreasing sequence (ε_ν) of positive reals tending to 0, as $\nu \rightarrow \infty$.

This topology is *not metrizable*, because the sets of sequences (m) and (ε) are essentially uncountable. It can, however, be shown to be the *inductive limit* of the topology of the subspaces \mathcal{Q}_K , in the following sense: V is a neighbourhood of the origin in \mathcal{Q} if and only if its intersection with \mathcal{Q}_K is a neighbourhood of the origin in \mathcal{Q}_K for any given compact K in Ω .

A sequence (φ_ν) in \mathcal{Q} will thus be said to converge to 0 in \mathcal{Q} if all the φ_ν belong to some \mathcal{Q}_K (with K a compact subset of Ω independent of ν) and if (φ_ν) converges to 0 in \mathcal{Q}_K .

As a result, a complex-valued functional T on \mathcal{Q} will be said to be continuous for the topology of \mathcal{Q} if and only if, for any given compact K in Ω , its restriction to \mathcal{Q}_K is continuous for the topology of \mathcal{Q}_K , *i.e.* maps convergent sequences in \mathcal{Q}_K to convergent sequences in \mathbb{C} .

This property of \mathcal{Q} , *i.e.* having a non-metrizable topology which is the inductive limit of metrizable topologies in its subspaces \mathcal{Q}_K , conditions the whole structure of distribution theory and dictates that of many of its proofs.

1.3.2.3.3.4. Topologies on $\mathcal{E}^{(m)}$, $\mathcal{Q}_K^{(m)}$, $\mathcal{Q}^{(m)}$

These are defined similarly, but only involve conditions on derivatives up to order m .

1.3.2.3.4. Definition of distributions

A *distribution* T on Ω is a *linear form* over $\mathcal{Q}(\Omega)$, *i.e.* a map

$$T : \varphi \mapsto \langle T, \varphi \rangle$$

which associates linearly a complex number $\langle T, \varphi \rangle$ to any $\varphi \in \mathcal{Q}(\Omega)$, and which is *continuous* for the topology of that space. In the terminology of Section 1.3.2.2.6.2, T is an element of $\mathcal{Q}'(\Omega)$, the *topological dual* of $\mathcal{Q}(\Omega)$.

Continuity over \mathcal{Q} is equivalent to continuity over \mathcal{Q}_K for all compact K contained in Ω , and hence to the condition that for any sequence (φ_ν) in \mathcal{Q} such that

- (i) $\text{Supp } \varphi_\nu$ is contained in some compact K independent of ν ,
- (ii) the sequences $(|D^{\mathbf{p}}\varphi_\nu|)$ converge uniformly to 0 on K for all multi-indices \mathbf{p} ;

then the sequence of complex numbers $\langle T, \varphi_\nu \rangle$ converges to 0 in \mathbb{C} .

If the continuity of a distribution T requires (ii) for $|\mathbf{p}| \leq m$ only, T may be defined over $\mathcal{Q}^{(m)}$ and thus $T \in \mathcal{Q}'^{(m)}$; T is said to be a *distribution of finite order* m . In particular, for $m = 0$, $\mathcal{Q}^{(0)}$ is the space of continuous functions with compact support, and a distribution $T \in \mathcal{Q}'^{(0)}$ is a (Radon) *measure* as used in the theory of integration. Thus measures are particular cases of distributions.

Generally speaking, the *larger* a space of test functions, the *smaller* its topological dual:

$$m < n \Rightarrow \mathcal{Q}^{(m)} \supset \mathcal{Q}^{(n)} \Rightarrow \mathcal{Q}'^{(n)} \supset \mathcal{Q}'^{(m)}.$$

This clearly results from the observation that if the φ 's are allowed to be less regular, then less wildness can be accommodated in T if the continuity of the map $\varphi \mapsto \langle T, \varphi \rangle$ with respect to φ is to be preserved.

1.3.2.3.5. First examples of distributions

(i) The linear map $\varphi \mapsto \langle \delta, \varphi \rangle = \varphi(\mathbf{0})$ is a measure (*i.e.* a zeroth-order distribution) called Dirac's measure or (improperly) Dirac's ' δ -function'.

(ii) The linear map $\varphi \mapsto \langle \delta_{(\mathbf{a})}, \varphi \rangle = \varphi(\mathbf{a})$ is called Dirac's measure at point $\mathbf{a} \in \mathbb{R}^n$.

(iii) The linear map $\varphi \mapsto (-1)^{|\mathbf{p}|} D^{\mathbf{p}}\varphi(\mathbf{a})$ is a distribution of order $m = |\mathbf{p}| > 0$, and hence is not a measure.

(iv) The linear map $\varphi \mapsto \sum_{\nu > 0} \varphi^{(\nu)}(\nu)$ is a distribution of infinite order on \mathbb{R} : the order of differentiation is bounded for each φ (because φ has compact support) but is not as φ varies.

(v) If (\mathbf{p}_ν) is a sequence of multi-indices $\mathbf{p}_\nu = (p_{1\nu}, \dots, p_{n\nu})$ such that $|\mathbf{p}_\nu| \rightarrow \infty$ as $\nu \rightarrow \infty$, then the linear map $\varphi \mapsto \sum_{\nu > 0} (D^{\mathbf{p}_\nu}\varphi)(\mathbf{p}_\nu)$ is a distribution of infinite order on \mathbb{R}^n .

1.3.2.3.6. Distributions associated to locally integrable functions

Let f be a complex-valued function over Ω such that $\int_K |f(\mathbf{x})| d^n \mathbf{x}$ exists for any given compact K in Ω ; f is then called *locally integrable*.

The linear mapping from $\mathcal{Q}(\Omega)$ to \mathbb{C} defined by

$$\varphi \mapsto \int_{\Omega} f(\mathbf{x})\varphi(\mathbf{x}) d^n \mathbf{x}$$

may then be shown to be continuous over $\mathcal{Q}(\Omega)$. It thus defines a *distribution* $T_f \in \mathcal{Q}'(\Omega)$:

$$\langle T_f, \varphi \rangle = \int_{\Omega} f(\mathbf{x})\varphi(\mathbf{x}) d^n \mathbf{x}.$$

As the continuity of T_f only requires that $\varphi \in \mathcal{Q}^{(0)}(\Omega)$, T_f is actually a Radon measure.