

1. GENERAL RELATIONSHIPS AND TECHNIQUES

objects (especially  $\delta$ -functions, their derivatives, their tensor products, their products with smooth functions, their translates and lattices of these translates), distribution theory can deal with all the major properties of the Fourier transformation as particular instances of a single basic result (the exchange between multiplication and convolution), and can at the same time accommodate the three previously distinct types of Fourier theories within a unique framework. This brings great simplification to matters of central importance in crystallography, such as the relations between

- (a) periodization, and sampling or decimation;
- (b) Shannon interpolation, and masking by an indicator function;
- (c) section, and projection;
- (d) differentiation, and multiplication by a monomial;
- (e) translation, and phase shift.

All these properties become subsumed under the same theorem. This striking synthesis comes at a slight price, which is the relative complexity of the notion of distribution. It is first necessary to establish the notion of topological vector space and to gain sufficient control (or, at least, understanding) over convergence behaviour in certain of these spaces. The key notion of *metrizability* cannot be circumvented, as it underlies most of the constructs and many of the proof techniques used in distribution theory. Most of Section 1.3.2.2 builds up to the fundamental result at the end of Section 1.3.2.2.6.2, which is basic to the definition of a distribution in Section 1.3.2.3.4 and to all subsequent developments.

The reader mostly interested in applications will probably want to reach this section by starting with his or her favourite topic in Section 1.3.4, and following the backward references to the relevant properties of the Fourier transformation, then to the proof of these properties, and finally to the definitions of the objects involved. Hopefully, he or she will then feel inclined to follow the forward references and thus explore the subject from the abstract to the practical. The books by Dieudonné (1969) and Lang (1965) are particularly recommended as general references for all aspects of analysis and algebra.

1.3.2.2. Preliminary notions and notation

Throughout this text,  $\mathbb{R}$  will denote the set of real numbers,  $\mathbb{Z}$  the set of rational (signed) integers and  $\mathbb{N}$  the set of natural (unsigned) integers. The symbol  $\mathbb{R}^n$  will denote the Cartesian product of  $n$  copies of  $\mathbb{R}$ :

$$\mathbb{R}^n = \mathbb{R} \times \dots \times \mathbb{R} \quad (n \text{ times}, n \geq 1),$$

so that an element  $\mathbf{x}$  of  $\mathbb{R}^n$  is an  $n$ -tuple of real numbers:

$$\mathbf{x} = (x_1, \dots, x_n).$$

Similar meanings will be attached to  $\mathbb{Z}^n$  and  $\mathbb{N}^n$ .

The symbol  $\mathbb{C}$  will denote the set of complex numbers. If  $z \in \mathbb{C}$ , its modulus will be denoted by  $|z|$ , its conjugate by  $\bar{z}$  (not  $z^*$ ), and its real and imaginary parts by  $\text{Re}(z)$  and  $\text{Im}(z)$ :

$$\text{Re}(z) = \frac{1}{2}(z + \bar{z}), \quad \text{Im}(z) = \frac{1}{2i}(z - \bar{z}).$$

If  $X$  is a finite set, then  $|X|$  will denote the number of its elements. If mapping  $f$  sends an element  $x$  of set  $X$  to the element  $f(x)$  of set  $Y$ , the notation

$$f : x \mapsto f(x)$$

will be used; the plain arrow  $\rightarrow$  will be reserved for denoting limits, as in

$$\lim_{\rho \rightarrow \infty} \left(1 + \frac{x}{\rho}\right)^\rho = e^x.$$

If  $X$  is any set and  $S$  is a subset of  $X$ , the *indicator function*  $\chi_S$  of  $S$  is the real-valued function on  $X$  defined by

$$\begin{aligned} \chi_S(x) &= 1 && \text{if } x \in S \\ &= 0 && \text{if } x \notin S. \end{aligned}$$

1.3.2.2.1. Metric and topological notions in  $\mathbb{R}^n$

The set  $\mathbb{R}^n$  can be endowed with the structure of a vector space of dimension  $n$  over  $\mathbb{R}$ , and can be made into a Euclidean space by treating its standard basis as an orthonormal basis and defining the Euclidean norm:

$$\|\mathbf{x}\| = \left(\sum_{i=1}^n x_i^2\right)^{1/2}.$$

By misuse of notation,  $\mathbf{x}$  will sometimes also designate the column vector of coordinates of  $\mathbf{x} \in \mathbb{R}^n$ ; if these coordinates are referred to an orthonormal basis of  $\mathbb{R}^n$ , then

$$\|\mathbf{x}\| = (\mathbf{x}^T \mathbf{x})^{1/2},$$

where  $\mathbf{x}^T$  denotes the transpose of  $\mathbf{x}$ .

The distance between two points  $\mathbf{x}$  and  $\mathbf{y}$  defined by  $d(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|$  allows the topological structure of  $\mathbb{R}$  to be transferred to  $\mathbb{R}^n$ , making it a *metric space*. The basic notions in a metric space are those of neighbourhoods, of open and closed sets, of limit, of continuity, and of convergence (see Section 1.3.2.2.6.1).

A subset  $S$  of  $\mathbb{R}^n$  is *bounded* if  $\sup \|\mathbf{x} - \mathbf{y}\| < \infty$  as  $\mathbf{x}$  and  $\mathbf{y}$  run through  $S$ ; it is *closed* if it contains the limits of all convergent sequences with elements in  $S$ . A subset  $K$  of  $\mathbb{R}^n$  which is both bounded and closed has the property of being *compact*, i.e. that whenever  $K$  has been covered by a family of open sets, a finite subfamily can be found which suffices to cover  $K$ . Compactness is a very useful topological property for the purpose of proof, since it allows one to reduce the task of examining infinitely many local situations to that of examining only finitely many of them.

1.3.2.2.2. Functions over  $\mathbb{R}^n$

Let  $\varphi$  be a complex-valued function over  $\mathbb{R}^n$ . The *support* of  $\varphi$ , denoted  $\text{Supp } \varphi$ , is the smallest closed subset of  $\mathbb{R}^n$  outside which  $\varphi$  vanishes identically. If  $\text{Supp } \varphi$  is compact,  $\varphi$  is said to have compact support.

If  $\mathbf{t} \in \mathbb{R}^n$ , the *translate* of  $\varphi$  by  $\mathbf{t}$ , denoted  $\tau_{\mathbf{t}}\varphi$ , is defined by

$$(\tau_{\mathbf{t}}\varphi)(\mathbf{x}) = \varphi(\mathbf{x} - \mathbf{t}).$$

Its support is the geometric translate of that of  $\varphi$ :

$$\text{Supp } \tau_{\mathbf{t}}\varphi = \{\mathbf{x} + \mathbf{t} \mid \mathbf{x} \in \text{Supp } \varphi\}.$$

If  $A$  is a non-singular linear transformation in  $\mathbb{R}^n$ , the *image* of  $\varphi$  by  $A$ , denoted  $A^\# \varphi$ , is defined by

$$(A^\# \varphi)(\mathbf{x}) = \varphi[A^{-1}(\mathbf{x})].$$

Its support is the geometric image of  $\text{Supp } \varphi$  under  $A$ :

$$\text{Supp } A^\# \varphi = \{A(\mathbf{x}) \mid \mathbf{x} \in \text{Supp } \varphi\}.$$

If  $S$  is a non-singular affine transformation in  $\mathbb{R}^n$  of the form

$$S(\mathbf{x}) = A(\mathbf{x}) + \mathbf{b}$$

with  $A$  linear, the image of  $\varphi$  by  $S$  is  $S^\# \varphi = \tau_{\mathbf{b}}(A^\# \varphi)$ , i.e.

$$(S^\# \varphi)(\mathbf{x}) = \varphi[A^{-1}(\mathbf{x} - \mathbf{b})].$$

Its support is the geometric image of  $\text{Supp } \varphi$  under  $S$ :

$$\text{Supp } S^\# \varphi = \{S(\mathbf{x}) \mid \mathbf{x} \in \text{Supp } \varphi\}.$$

It may be helpful to visualize the process of forming the image of a function by a geometric operation as consisting of applying that operation to the *graph* of that function, which is equivalent to

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applying the *inverse* transformation to the coordinates  $\mathbf{x}$ . This use of the inverse later affords the ‘left-representation property’ [see Section 1.3.4.2.2.2(e)] when the geometric operations form a group, which is of fundamental importance in the treatment of crystallographic symmetry (Sections 1.3.4.2.2.4, 1.3.4.2.2.5).

#### 1.3.2.2.3. Multi-index notation

When dealing with functions in  $n$  variables and their derivatives, considerable abbreviation of notation can be obtained through the use of multi-indices.

A *multi-index*  $\mathbf{p} \in \mathbb{N}^n$  is an  $n$ -tuple of natural integers:  $\mathbf{p} = (p_1, \dots, p_n)$ . The *length* of  $\mathbf{p}$  is defined as

$$|\mathbf{p}| = \sum_{i=1}^n p_i,$$

and the following abbreviations will be used:

- (i)  $\mathbf{x}^{\mathbf{p}} = x_1^{p_1} \dots x_n^{p_n}$
- (ii)  $D_i f = \frac{\partial f}{\partial x_i} = \partial_i f$
- (iii)  $D^{\mathbf{p}} f = D_1^{p_1} \dots D_n^{p_n} f = \frac{\partial^{|\mathbf{p}|} f}{\partial x_1^{p_1} \dots \partial x_n^{p_n}}$
- (iv)  $\mathbf{q} \leq \mathbf{p}$  if and only if  $q_i \leq p_i$  for all  $i = 1, \dots, n$
- (v)  $\mathbf{p} - \mathbf{q} = (p_1 - q_1, \dots, p_n - q_n)$
- (vi)  $\mathbf{p}! = p_1! \times \dots \times p_n!$
- (vii)  $\binom{\mathbf{p}}{\mathbf{q}} = \binom{p_1}{q_1} \times \dots \times \binom{p_n}{q_n}$ .

Leibniz’s formula for the repeated differentiation of products then assumes the concise form

$$D^{\mathbf{p}}(fg) = \sum_{\mathbf{q} \leq \mathbf{p}} \binom{\mathbf{p}}{\mathbf{q}} D^{\mathbf{p}-\mathbf{q}} f D^{\mathbf{q}} g,$$

while the Taylor expansion of  $f$  to order  $m$  about  $\mathbf{x} = \mathbf{a}$  reads

$$f(\mathbf{x}) = \sum_{|\mathbf{p}| \leq m} \frac{1}{\mathbf{p}!} [D^{\mathbf{p}} f(\mathbf{a})] (\mathbf{x} - \mathbf{a})^{\mathbf{p}} + o(\|\mathbf{x} - \mathbf{a}\|^m).$$

In certain sections the notation  $\nabla f$  will be used for the gradient vector of  $f$ , and the notation  $(\nabla \nabla^T) f$  for the Hessian matrix of its mixed second-order partial derivatives:

$$\nabla = \begin{pmatrix} \frac{\partial}{\partial x_1} \\ \vdots \\ \frac{\partial}{\partial x_n} \end{pmatrix}, \quad \nabla f = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix},$$

$$(\nabla \nabla^T) f = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{pmatrix}.$$

#### 1.3.2.2.4. Integration, $L^p$ spaces

The Riemann integral used in elementary calculus suffers from the drawback that vector spaces of Riemann-integrable functions over  $\mathbb{R}^n$  are not *complete* for the topology of convergence in the

mean: a Cauchy sequence of integrable functions may converge to a non-integrable function.

To obtain the property of completeness, which is fundamental in functional analysis, it was necessary to extend the notion of integral. This was accomplished by Lebesgue [see Berberian (1962), Dieudonné (1970), or Chapter 1 of Dym & McKean (1972) and the references therein, or Chapter 9 of Sprecher (1970)], and entailed identifying functions which differed only on a subset of zero measure in  $\mathbb{R}^n$  (such functions are said to be equal ‘almost everywhere’). The vector spaces  $L^p(\mathbb{R}^n)$  consisting of function classes  $f$  modulo this identification for which

$$\|f\|_p = \left( \int_{\mathbb{R}^n} |f(\mathbf{x})|^p d^n \mathbf{x} \right)^{1/p} < \infty$$

are then complete for the topology induced by the norm  $\|\cdot\|_p$ : the limit of every Cauchy sequence of functions in  $L^p$  is itself a function in  $L^p$  (Riesz–Fischer theorem).

The space  $L^1(\mathbb{R}^n)$  consists of those function classes  $f$  such that

$$\|f\|_1 = \int_{\mathbb{R}^n} |f(\mathbf{x})| d^n \mathbf{x} < \infty$$

which are called *summable* or *absolutely integrable*. The convolution product:

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

is well defined; combined with the vector space structure of  $L^1$ , it makes  $L^1$  into a (commutative) *convolution algebra*. However, this algebra has no unit element: there is no  $f \in L^1$  such that  $f * g = g$  for all  $g \in L^1$ ; it has only approximate units, *i.e.* sequences  $(f_\nu)$  such that  $f_\nu * g$  tends to  $g$  in the  $L^1$  topology as  $\nu \rightarrow \infty$ . This is one of the starting points of distribution theory.

The space  $L^2(\mathbb{R}^n)$  of *square-integrable* functions can be endowed with a scalar product

$$(f, g) = \int_{\mathbb{R}^n} \overline{f(\mathbf{x})} g(\mathbf{x}) d^n \mathbf{x}$$

which makes it into a *Hilbert space*. The Cauchy–Schwarz inequality

$$|(f, g)| \leq [(f, f)(g, g)]^{1/2}$$

generalizes the fact that the absolute value of the cosine of an angle is less than or equal to 1.

The space  $L^\infty(\mathbb{R}^n)$  is defined as the space of functions  $f$  such that

$$\|f\|_\infty = \lim_{p \rightarrow \infty} \|f\|_p = \lim_{p \rightarrow \infty} \left( \int_{\mathbb{R}^n} |f(\mathbf{x})|^p d^n \mathbf{x} \right)^{1/p} < \infty.$$

The quantity  $\|f\|_\infty$  is called the ‘essential sup norm’ of  $f$ , as it is the smallest positive number which  $|f(\mathbf{x})|$  exceeds only on a subset of zero measure in  $\mathbb{R}^n$ . A function  $f \in L^\infty$  is called *essentially bounded*.

#### 1.3.2.2.5. Tensor products. Fubini’s theorem

Let  $f \in L^1(\mathbb{R}^m)$ ,  $g \in L^1(\mathbb{R}^n)$ . Then the function

$$f \otimes g : (\mathbf{x}, \mathbf{y}) \mapsto f(\mathbf{x})g(\mathbf{y})$$

is called the *tensor product* of  $f$  and  $g$ , and belongs to  $L^1(\mathbb{R}^m \times \mathbb{R}^n)$ . The finite linear combinations of functions of the form  $f \otimes g$  span a subspace of  $L^1(\mathbb{R}^m \times \mathbb{R}^n)$  called the tensor product of  $L^1(\mathbb{R}^m)$  and  $L^1(\mathbb{R}^n)$  and denoted  $L^1(\mathbb{R}^m) \otimes L^1(\mathbb{R}^n)$ .