

1. GENERAL RELATIONSHIPS AND TECHNIQUES

If $\mathbf{t} \in \mathbb{R}^n$, the *translate* of φ 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 φ :

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

If A is a nonsingular linear transformation in \mathbb{R}^n , the *image* of φ 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 :

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

If S is a nonsingular affine transformation in \mathbb{R}^n of the form

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

with A linear, the image of φ 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 :

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

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 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 ∇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 nonintegrable 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

1.3. FOURIER TRANSFORMS IN CRYSTALLOGRAPHY

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

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_ν) 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 $L^1(\mathbb{R}^m) \otimes L^1(\mathbb{R}^n)$.

The integration of a general function over $\mathbb{R}^m \times \mathbb{R}^n$ may be accomplished in two steps according to *Fubini’s theorem*. Given $F \in L^1(\mathbb{R}^m \times \mathbb{R}^n)$, the functions

$$F_1 : \mathbf{x} \mapsto \int_{\mathbb{R}^n} F(\mathbf{x}, \mathbf{y}) d^n \mathbf{y}$$

$$F_2 : \mathbf{y} \mapsto \int_{\mathbb{R}^m} F(\mathbf{x}, \mathbf{y}) d^m \mathbf{x}$$

exist for almost all $\mathbf{x} \in \mathbb{R}^m$ and almost all $\mathbf{y} \in \mathbb{R}^n$, respectively, are integrable, and

$$\int_{\mathbb{R}^m \times \mathbb{R}^n} F(\mathbf{x}, \mathbf{y}) d^m \mathbf{x} d^n \mathbf{y} = \int_{\mathbb{R}^m} F_1(\mathbf{x}) d^m \mathbf{x} = \int_{\mathbb{R}^n} F_2(\mathbf{y}) d^n \mathbf{y}.$$

Conversely, if any one of the integrals

- (i) $\int_{\mathbb{R}^m \times \mathbb{R}^n} |F(\mathbf{x}, \mathbf{y})| d^m \mathbf{x} d^n \mathbf{y}$
- (ii) $\int_{\mathbb{R}^m} \left(\int_{\mathbb{R}^n} |F(\mathbf{x}, \mathbf{y})| d^n \mathbf{y} \right) d^m \mathbf{x}$
- (iii) $\int_{\mathbb{R}^n} \left(\int_{\mathbb{R}^m} |F(\mathbf{x}, \mathbf{y})| d^m \mathbf{x} \right) d^n \mathbf{y}$

is finite, then so are the other two, and the identity above holds. It is then (and only then) permissible to change the order of integrations.

Fubini’s theorem is of fundamental importance in the study of tensor products and convolutions of distributions.

1.3.2.2.6. Topology in function spaces

Geometric intuition, which often makes ‘obvious’ the topological properties of the real line and of ordinary space, cannot be relied upon in the study of function spaces: the latter are infinite-dimensional, and several inequivalent notions of convergence may exist. A careful analysis of topological concepts and of their interrelationship is thus a necessary prerequisite to the study of these spaces. The reader may consult Dieudonné (1969, 1970), Friedman (1970), Trèves (1967) and Yosida (1965) for detailed expositions.

1.3.2.2.6.1. General topology

Most topological notions are first encountered in the setting of *metric spaces*. A metric space E is a set equipped with a *distance function* d from $E \times E$ to the non-negative reals which satisfies:

- (i) $d(x, y) = d(y, x) \quad \forall x, y \in E$ (symmetry);
- (ii) $d(x, y) = 0$ iff $x = y$ (separation);
- (iii) $d(x, z) \leq d(x, y) + d(y, z) \quad \forall x, y, z \in E$ (triangular inequality).

By means of d , the following notions can be defined: open balls, neighbourhoods; open and closed sets, interior and closure; convergence of sequences, continuity of mappings; Cauchy sequences and completeness; compactness; connectedness. They suffice for the investigation of a great number of questions in analysis and geometry (see *e.g.* Dieudonné, 1969).

Many of these notions turn out to depend only on the properties of the collection $\mathcal{O}(E)$ of open subsets of E : two distance functions leading to the same $\mathcal{O}(E)$ lead to identical topological properties. An axiomatic reformulation of topological notions is thus possible: a *topology* in E is a collection $\mathcal{O}(E)$ of subsets of E which satisfy suitable axioms and are deemed open irrespective