International Tables for Crystallography (2006). Vol. B, Section 1.3.2.2.5, pp. 27–28.

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: $\mathbf{p} = (p_1, \ldots, p_n)$. The *length* of $\mathbf{p}$ is defined as

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

and the following abbreviations will be used:

(i) $\mathbf{x}^{\mathbf{p}} = x_1^{p_1} \ldots x_n^{p_n}$

(ii) $D_i f = \dfrac{\partial f}{\partial x_i} = \partial_i f$

(iii) $D^{\mathbf{p}} f = D_1^{p_1} \ldots D_n^{p_n} f = \dfrac{\partial^{|\mathbf{p}|} f}{\partial x_1^{p_1} \ldots \partial x_n^{p_n}}$

(iv) $\mathbf{q} \leq \mathbf{p}$ if and only if $q_i \leq p_i$ for all $i = 1, \ldots, n$

(v) $\mathbf{p} - \mathbf{q} = (p_1 - q_1, \ldots, p_n - q_n)$

(vi) $\mathbf{p}! = p_1! \times \ldots \times p_n!$

(vii) $\begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix} = \begin{pmatrix} p_1 \\ q_1 \end{pmatrix} \times \ldots \times \begin{pmatrix} p_n \\ q_n \end{pmatrix}.$

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

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

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:

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

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

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

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

are then complete for the topology induced by the norm $\|.\|_p$: 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

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

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

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

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 $\nu \to \infty$. 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

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

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

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

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

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

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

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

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

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

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

Conversely, if any one of the integrals

(i) $\displaystyle\int_{\mathbb{R}^m \times \mathbb{R}^n} |F(\mathbf{x}, \mathbf{y})|\, \mathrm{d}^m\mathbf{x}\, \mathrm{d}^n\mathbf{y}$

(ii) $\displaystyle\int_{\mathbb{R}^m} \left(\int_{\mathbb{R}^n} |F(\mathbf{x}, \mathbf{y})|\, \mathrm{d}^n\mathbf{y} \right) \mathrm{d}^m\mathbf{x}$

(iii) $\displaystyle\int_{\mathbb{R}^n} \left(\int_{\mathbb{R}^m} |F(\mathbf{x}, \mathbf{y})|\, \mathrm{d}^m\mathbf{x} \right) \mathrm{d}^n\mathbf{y}$

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)	$d(x, y) = d(y, x)$	$\forall x, y \in E$	(symmetry);
(ii)	$d(x, y) = 0$	iff $x = y$	(separation);
(iii)	$d(x, z) \leq d(x, y) + d(y, z)$	$\forall x, y, z \in E$	(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 of the way they are obtained. From the practical standpoint, however, a topology which can be obtained from a distance function (called a *metrizable* topology) has the very useful property that *the notions of closure, limit and continuity may be defined by means of sequences*. For non-metrizable topologies, these notions are much more difficult to handle, requiring the use of 'filters' instead of sequences.

In some spaces E, a topology may be most naturally defined by a family of *pseudo-distances* $(d_\alpha)_{\alpha \in A}$, where each d_α satisfies (i) and (iii) but not (ii). Such spaces are called *uniformizable*. If for every pair $(x, y) \in E \times E$ there exists $\alpha \in A$ such that $d_\alpha(x, y) \neq 0$, then the separation property can be recovered. If furthermore a *countable* subfamily of the d_α suffices to define the topology of E, the latter can be shown to be *metrizable*, so that limiting processes in E may be studied by means of sequences.

1.3.2.2.6.2. *Topological vector spaces*

The function spaces E of interest in Fourier analysis have an underlying vector space structure over the field $\mathbb{C}$ of complex numbers. A topology on E is said to be *compatible* with a vector space structure on E if vector addition [*i.e.* the map $(\mathbf{x}, \mathbf{y}) \longmapsto \mathbf{x} + \mathbf{y}$] and scalar multiplication [*i.e.* the map $(\lambda, \mathbf{x}) \longmapsto \lambda\mathbf{x}$] are both *continuous*; E is then called a *topological vector space*. Such a topology may be defined by specifying a 'fundamental system S of neighbourhoods of $\mathbf{0}$', which can then be translated by vector addition to construct neighbourhoods of other points $\mathbf{x} \neq \mathbf{0}$.

A *norm* ν on a vector space E is a non-negative real-valued function on $E \times E$ such that

(i′)	$\nu(\lambda\mathbf{x}) = \lvert\lambda\rvert\nu(\mathbf{x})$	for all $\lambda \in \mathbb{C}$ and $\mathbf{x} \in E$;
(ii′)	$\nu(\mathbf{x}) = 0$	if and only if $\mathbf{x} = \mathbf{0}$;
(iii′)	$\nu(\mathbf{x} + \mathbf{y}) \leq \nu(\mathbf{x}) + \nu(\mathbf{y})$	for all $\mathbf{x}, \mathbf{y} \in E$.

Subsets of E defined by conditions of the form $\nu(\mathbf{x}) \leq r$ with $r > 0$ form a fundamental system of neighbourhoods of $\mathbf{0}$. The corresponding topology makes E a *normed space*. This topology is *metrizable*, since it is equivalent to that derived from the translation-invariant distance $d(\mathbf{x}, \mathbf{y}) = \nu(\mathbf{x} - \mathbf{y})$. Normed spaces which are *complete*, *i.e.* in which all Cauchy sequences converge, are called *Banach spaces*; they constitute the natural setting for the study of differential calculus.

A *semi-norm* σ on a vector space E is a positive real-valued function on $E \times E$ which satisfies (i′) and (iii′) but not (ii′). Given a set Σ of semi-norms on E such that any pair $(\mathbf{x}, \mathbf{y})$ in $E \times E$ is separated by at least one $\sigma \in \Sigma$, let B be the set of those subsets $\Gamma_{\sigma, r}$ of E defined by a condition of the form $\sigma(\mathbf{x}) \leq r$ with $\sigma \in \Sigma$ and $r > 0$; and let S be the set of finite intersections of elements of B. Then there exists a unique topology on E for which S is a fundamental system of neighbourhoods of $\mathbf{0}$. This topology is *uniformizable* since it is equivalent to that derived from the family of translation-invariant pseudo-distances $(\mathbf{x}, \mathbf{y}) \longmapsto \sigma(\mathbf{x} - \mathbf{y})$. It is *metrizable* if and only if it can be constructed by the above procedure with Σ a *countable* set of semi-norms. If furthermore E is complete, E is called a *Fréchet space*.

If E is a topological vector space over $\mathbb{C}$, its *dual* E^* is the set of all linear mappings from E to $\mathbb{C}$ (which are also called *linear forms*, or *linear functionals*, over E). The subspace of E^* consisting of all linear forms which are *continuous* for the topology of E is called the *topological dual* of E and is denoted E'. If the topology on E is metrizable, then the continuity of a linear form $T \in E'$ at $f \in E$ can be ascertained by means of sequences, *i.e.* by checking that the sequence $[T(f_j)]$ of complex numbers converges to $T(f)$ in $\mathbb{C}$ whenever the sequence (f_j) converges to f in E.

1.3.2.3. *Elements of the theory of distributions*

1.3.2.3.1. *Origins*

At the end of the 19th century, Heaviside proposed under the name of 'operational calculus' a set of rules for solving a class of

references