

1.3. FOURIER TRANSFORMS IN CRYSTALLOGRAPHY

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:

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

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

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