

1. GENERAL RELATIONSHIPS AND TECHNIQUES

$$\begin{aligned} \mathcal{F}[\delta_{\mathbf{x}}^{(\mathbf{m})}]_{\xi} &= (2\pi i \xi)^{\mathbf{m}}, & \mathcal{F}[\mathbf{x}^{\mathbf{m}}]_{\xi} &= (-2\pi i)^{-|\mathbf{m}|} \delta_{\xi}^{(\mathbf{m})}; \\ \mathcal{F}[\delta_{\mathbf{a}}]_{\xi} &= \exp(-2\pi i \mathbf{a} \cdot \xi), & \mathcal{F}[\exp(2\pi i \boldsymbol{\alpha} \cdot \mathbf{x})]_{\xi} &= \delta_{\boldsymbol{\alpha}}, \end{aligned}$$

with analogous relations for $\tilde{\mathcal{F}}$, i becoming $-i$. Thus derivatives of δ are mapped to monomials (and *vice versa*), while translates of δ are mapped to ‘phase factors’ (and *vice versa*).

1.3.2.5.7. Reciprocity theorem

The previous results now allow a self-contained and rigorous proof of the reciprocity theorem between \mathcal{F} and $\tilde{\mathcal{F}}$ to be given, whereas in traditional settings (*i.e.* in L^1 and L^2) the implicit handling of δ through a limiting process is always the sticking point.

Reciprocity is first established in \mathcal{S} as follows:

$$\begin{aligned} \tilde{\mathcal{F}}[\mathcal{F}[\varphi]](\mathbf{x}) &= \int_{\mathbb{R}^n} \mathcal{F}[\varphi](\xi) \exp(2\pi i \xi \cdot \mathbf{x}) d^n \xi \\ &= \int_{\mathbb{R}^n} \mathcal{F}[\tau_{-\mathbf{x}}\varphi](\xi) d^n \xi \\ &= \langle 1, \mathcal{F}[\tau_{-\mathbf{x}}\varphi] \rangle \\ &= \langle \mathcal{F}[1], \tau_{-\mathbf{x}}\varphi \rangle \\ &= \langle \tau_{\mathbf{x}}\delta, \varphi \rangle \\ &= \varphi(\mathbf{x}) \end{aligned}$$

and similarly

$$\mathcal{F}[\tilde{\mathcal{F}}[\varphi]](\mathbf{x}) = \varphi(\mathbf{x}).$$

The reciprocity theorem is then proved in \mathcal{S}' by transposition:

$$\tilde{\mathcal{F}}[\mathcal{F}[T]] = \mathcal{F}[\tilde{\mathcal{F}}[T]] = T \quad \text{for all } T \in \mathcal{S}'.$$

Thus the Fourier cotransformation $\tilde{\mathcal{F}}$ in \mathcal{S}' may legitimately be called the ‘inverse Fourier transformation’.

The method of Section 1.3.2.4.3 may then be used to show that $\tilde{\mathcal{F}}$ and \mathcal{F} both have period 4 in \mathcal{S}' .

1.3.2.5.8. Multiplication and convolution

Multiplier functions $\alpha(\mathbf{x})$ for tempered distributions must be infinitely differentiable, as for ordinary distributions; furthermore, they must grow sufficiently slowly as $\|\mathbf{x}\| \rightarrow \infty$ to ensure that $\alpha\varphi \in \mathcal{S}$ for all $\varphi \in \mathcal{S}$ and that the map $\varphi \mapsto \alpha\varphi$ is continuous for the topology of \mathcal{S} . This leads to choosing for multipliers the subspace \mathcal{O}_M consisting of functions $\alpha \in \mathcal{E}$ of polynomial growth. It can be shown that if f is in \mathcal{O}_M , then the associated distribution T_f is in \mathcal{S}' (*i.e.* is a tempered distribution); and that conversely if T is in \mathcal{S}' , $\mu * T$ is in \mathcal{O}_M for all $\mu \in \mathcal{D}$.

Corresponding restrictions must be imposed to define the space \mathcal{O}'_C of those distributions T whose convolution $S * T$ with a tempered distribution S is still a tempered distribution: T must be such that, for all $\varphi \in \mathcal{S}$, $\theta(\mathbf{x}) = \langle T_{\mathbf{y}}, \varphi(\mathbf{x} + \mathbf{y}) \rangle$ is in \mathcal{S} ; and such that the map $\varphi \mapsto \theta$ be continuous for the topology of \mathcal{S} . This implies that S is ‘rapidly decreasing’. It can be shown that if f is in \mathcal{S} , then the associated distribution T_f is in \mathcal{O}'_C ; and that conversely if T is in \mathcal{O}'_C , $\mu * T$ is in \mathcal{S} for all $\mu \in \mathcal{D}$.

The two spaces \mathcal{O}_M and \mathcal{O}'_C are mapped into each other by the Fourier transformation

$$\begin{aligned} \mathcal{F}(\mathcal{O}_M) &= \tilde{\mathcal{F}}(\mathcal{O}_M) = \mathcal{O}'_C \\ \mathcal{F}(\mathcal{O}'_C) &= \tilde{\mathcal{F}}(\mathcal{O}'_C) = \mathcal{O}_M \end{aligned}$$

and the convolution theorem takes the form

$$\begin{aligned} \mathcal{F}[\alpha S] &= \mathcal{F}[\alpha] * \mathcal{F}[S] & S \in \mathcal{S}', \alpha \in \mathcal{O}_M, \mathcal{F}[\alpha] \in \mathcal{O}'_C; \\ \mathcal{F}[S * T] &= \mathcal{F}[S] \times \mathcal{F}[T] & S \in \mathcal{S}', T \in \mathcal{O}'_C, \mathcal{F}[T] \in \mathcal{O}_M. \end{aligned}$$

The same identities hold for $\tilde{\mathcal{F}}$. Taken together with the reciprocity theorem, these show that \mathcal{F} and $\tilde{\mathcal{F}}$ establish mutually inverse isomorphisms between \mathcal{O}_M and \mathcal{O}'_C , and exchange multiplication for convolution in \mathcal{S}' .

It may be noticed that most of the basic properties of \mathcal{F} and $\tilde{\mathcal{F}}$ may be deduced from this theorem and from the properties of δ . Differentiation operators $D^{\mathbf{m}}$ and translation operators $\tau_{\mathbf{a}}$ are convolutions with $D^{\mathbf{m}}\delta$ and $\tau_{\mathbf{a}}\delta$; they are turned, respectively, into multiplication by monomials $(\pm 2\pi i \xi)^{\mathbf{m}}$ (the transforms of $D^{\mathbf{m}}\delta$) or by phase factors $\exp(\pm 2\pi i \xi \cdot \mathbf{a})$ (the transforms of $\tau_{\mathbf{a}}\delta$).

Another consequence of the convolution theorem is the duality established by the Fourier transformation between sections and projections of a function and its transform. For instance, in \mathbb{R}^3 , the projection of $f(x, y, z)$ on the x, y plane along the z axis may be written

$$(\delta_x \otimes \delta_y \otimes 1_z) * f;$$

its Fourier transform is then

$$(1_{\xi} \otimes 1_{\eta} \otimes \delta_{\zeta}) \times \mathcal{F}[f],$$

which is the section of $\mathcal{F}[f]$ by the plane $\zeta = 0$, orthogonal to the z axis used for projection. There are numerous applications of this property in crystallography (Section 1.3.4.2.1.8) and in fibre diffraction (Section 1.3.4.5.1.3).

1.3.2.5.9. L^2 aspects, Sobolev spaces

The special properties of \mathcal{F} in the space of square-integrable functions $L^2(\mathbb{R}^n)$, such as Parseval’s identity, can be accommodated within distribution theory: if $u \in L^2(\mathbb{R}^n)$, then T_u is a tempered distribution in \mathcal{S}' (the map $u \mapsto T_u$ being continuous) and it can be shown that $S = \mathcal{F}[T_u]$ is of the form S_v , where $u = \mathcal{F}[u]$ is the Fourier transform of u in $L^2(\mathbb{R}^n)$. By Plancherel’s theorem, $\|u\|_2 = \|v\|_2$.

This embedding of L^2 into \mathcal{S}' can be used to derive the convolution theorem for L^2 . If u and v are in $L^2(\mathbb{R}^n)$, then $u * v$ can be shown to be a bounded continuous function; thus $u * v$ is not in L^2 , but it is in \mathcal{S}' , so that its Fourier transform is a distribution, and

$$\mathcal{F}[u * v] = \mathcal{F}[u] \times \mathcal{F}[v].$$

Spaces of tempered distributions related to $L^2(\mathbb{R}^n)$ can be defined as follows. For any real s , define the Sobolev space $H_s(\mathbb{R}^n)$ to consist of all tempered distributions $S \in \mathcal{S}'(\mathbb{R}^n)$ such that

$$(1 + |\xi|^2)^{s/2} \mathcal{F}[S]_{\xi} \in L^2(\mathbb{R}^n).$$

These spaces play a fundamental role in the theory of partial differential equations, and in the mathematical theory of tomographic reconstruction – a subject not unrelated to the crystallographic phase problem (Natterer, 1986).

1.3.2.6. Periodic distributions and Fourier series

1.3.2.6.1. Terminology

Let \mathbb{Z}^n be the subset of \mathbb{R}^n consisting of those points with (signed) integer coordinates; it is an n -dimensional lattice, *i.e.* a free Abelian group on n generators. A particularly simple set of n generators is given by the standard basis of \mathbb{R}^n , and hence \mathbb{Z}^n will be called the standard lattice in \mathbb{R}^n . Any other ‘non-standard’ n -dimensional lattice Λ in \mathbb{R}^n is the image of this standard lattice by a general linear transformation.

If we identify any two points in \mathbb{R}^n whose coordinates are congruent modulo \mathbb{Z}^n , *i.e.* differ by a vector in \mathbb{Z}^n , we obtain the standard n -torus $\mathbb{R}^n/\mathbb{Z}^n$. The latter may be viewed as $(\mathbb{R}/\mathbb{Z})^n$, *i.e.* as the Cartesian product of n circles. The same identification may be carried out modulo a non-standard lattice Λ , yielding a non-