

1. GENERAL RELATIONSHIPS AND TECHNIQUES

where \mathbf{A} is a symmetric positive-definite matrix. Diagonalizing \mathbf{A} as $\mathbf{E}\mathbf{A}\mathbf{E}^T$ with $\mathbf{E}\mathbf{E}^T$ the identity matrix, and putting $\mathbf{A}^{1/2} = \mathbf{E}\mathbf{A}^{1/2}\mathbf{E}^T$, we may write

$$G_{\mathbf{A}}(\mathbf{x}) = G \left[\left(\frac{\mathbf{A}}{2\pi} \right)^{1/2} \mathbf{x} \right]$$

i.e.

$$G_{\mathbf{A}} = [(2\pi\mathbf{A}^{-1})^{1/2}]^{\#} G;$$

hence (by Section 1.3.2.4.2.3)

$$\mathcal{F}[G_{\mathbf{A}}] = |\det(2\pi\mathbf{A}^{-1})|^{1/2} \left[\left(\frac{\mathbf{A}}{2\pi} \right)^{1/2} \right]^{\#} G,$$

i.e.

$$\mathcal{F}[G_{\mathbf{A}}](\boldsymbol{\xi}) = |\det(2\pi\mathbf{A}^{-1})|^{1/2} G[(2\pi\mathbf{A}^{-1})^{1/2}\boldsymbol{\xi}],$$

i.e. finally

$$\mathcal{F}[G_{\mathbf{A}}] = |\det(2\pi\mathbf{A}^{-1})|^{1/2} G_{4\pi^2\mathbf{A}^{-1}}.$$

This result is widely used in crystallography, *e.g.* to calculate form factors for anisotropic atoms (Section 1.3.4.2.2.6) and to obtain transforms of derivatives of Gaussian atomic densities (Section 1.3.4.4.7.10).

1.3.2.4.4.3. Heisenberg's inequality, Hardy's theorem

The result just obtained, which also holds for $\tilde{\mathcal{F}}$, shows that the 'peakier' $G_{\mathbf{A}}$, the 'broader' $\mathcal{F}[G_{\mathbf{A}}]$. This is a general property of the Fourier transformation, expressed in dimension 1 by the *Heisenberg inequality* (Weyl, 1931):

$$\left(\int x^2 |f(x)|^2 dx \right) \left(\int \xi^2 |\mathcal{F}[f](\xi)|^2 d\xi \right) \geq \frac{1}{16\pi^2} \left(\int |f(x)|^2 dx \right)^2,$$

where, by a beautiful theorem of Hardy (1933), equality can only be attained for f Gaussian. Hardy's theorem is even stronger: if both f and $\mathcal{F}[f]$ behave at infinity as constant multiples of G , then each of them is *everywhere* a constant multiple of G ; if both f and $\mathcal{F}[f]$ behave at infinity as constant multiples of $G \times$ monomial, then each of them is a finite linear combination of Hermite functions. Hardy's theorem is invoked in Section 1.3.4.4.5 to derive the optimal procedure for spreading atoms on a sampling grid in order to obtain the most accurate structure factors.

The search for optimal compromises between the confinement of f to a compact domain in x -space and of $\mathcal{F}[f]$ to a compact domain in ξ -space leads to consideration of prolate spheroidal wavefunctions (Pollack & Slepian, 1961; Landau & Pollack, 1961, 1962).

1.3.2.4.4.4. Symmetry property

A final formal property of the Fourier transform, best established in \mathcal{S} , is its *symmetry*: if f and g are in \mathcal{S} , then by Fubini's theorem

$$\begin{aligned} \langle \mathcal{F}[f], g \rangle &= \int_{\mathbb{R}^n} \left(\int_{\mathbb{R}^n} f(\mathbf{x}) \exp(-2\pi i \boldsymbol{\xi} \cdot \mathbf{x}) d^n \mathbf{x} \right) g(\boldsymbol{\xi}) d^n \boldsymbol{\xi} \\ &= \int_{\mathbb{R}^n} f(\mathbf{x}) \left(\int_{\mathbb{R}^n} g(\boldsymbol{\xi}) \exp(-2\pi i \boldsymbol{\xi} \cdot \mathbf{x}) d^n \boldsymbol{\xi} \right) d^n \mathbf{x} \\ &= \langle f, \mathcal{F}[g] \rangle. \end{aligned}$$

This possibility of 'transposing' \mathcal{F} (and $\tilde{\mathcal{F}}$) from the left to the right of the duality bracket will be used in Section 1.3.2.5.4 to extend the Fourier transformation to distributions.

1.3.2.4.5. Various writings of Fourier transforms

Other ways of writing Fourier transforms in \mathbb{R}^n exist besides the one used here. All have the form

$$\mathcal{F}_{h,\omega}[f](\boldsymbol{\xi}) = \frac{1}{h^n} \int_{\mathbb{R}^n} f(\mathbf{x}) \exp(-i\omega \boldsymbol{\xi} \cdot \mathbf{x}) d^n \mathbf{x},$$

where h is real positive and ω real non-zero, with the reciprocity formula written:

$$f(\mathbf{x}) = \frac{1}{k^n} \int_{\mathbb{R}^n} \mathcal{F}_{h,\omega}[f](\boldsymbol{\xi}) \exp(+i\omega \boldsymbol{\xi} \cdot \mathbf{x}) d^n \mathbf{x}$$

with k real positive. The consistency condition between h , k and ω is

$$hk = \frac{2\pi}{|\omega|}.$$

The usual choices are:

- (i) $\omega = \pm 2\pi, h = k = 1$ (as here);
- (ii) $\omega = \pm 1, h = 1, k = 2\pi$ (in probability theory and in solid-state physics);
- (iii) $\omega = \pm 1, h = k = \sqrt{2\pi}$ (in much of classical analysis).

It should be noted that conventions (ii) and (iii) introduce numerical factors of 2π in convolution and Parseval formulae, while (ii) breaks the symmetry between \mathcal{F} and $\tilde{\mathcal{F}}$.

1.3.2.4.6. Tables of Fourier transforms

The books by Campbell & Foster (1948), Erdélyi (1954), and Magnus *et al.* (1966) contain extensive tables listing pairs of functions and their Fourier transforms. Bracewell (1986) lists those pairs particularly relevant to electrical engineering applications.

1.3.2.5. Fourier transforms of tempered distributions

1.3.2.5.1. Introduction

It was found in Section 1.3.2.4.2 that the usual space of test functions \mathcal{D} is not invariant under \mathcal{F} and $\tilde{\mathcal{F}}$. By contrast, the space \mathcal{S} of infinitely differentiable rapidly decreasing functions is invariant under \mathcal{F} and $\tilde{\mathcal{F}}$, and furthermore transposition formulae such as

$$\langle \mathcal{F}[f], g \rangle = \langle f, \mathcal{F}[g] \rangle$$

hold for all $f, g \in \mathcal{S}$. It is precisely this type of transposition which was used successfully in Sections 1.3.2.3.9.1 and 1.3.2.3.9.3 to define the derivatives of distributions and their products with smooth functions.

This suggests using \mathcal{S} instead of \mathcal{D} as a space of test functions φ , and defining the Fourier transform $\mathcal{F}[T]$ of a distribution T by

$$\langle \mathcal{F}[T], \varphi \rangle = \langle T, \mathcal{F}[\varphi] \rangle$$

whenever T is capable of being extended from \mathcal{D} to \mathcal{S} while remaining continuous. It is this latter proviso which will be subsumed under the adjective 'tempered'. As was the case with the construction of \mathcal{S}' , it is the definition of a sufficiently strong topology (*i.e.* notion of convergence) in \mathcal{S} which will play a key role in transferring to the elements of its topological dual \mathcal{S}' (called tempered distributions) all the properties of the Fourier transformation.

1.3. FOURIER TRANSFORMS IN CRYSTALLOGRAPHY

Besides the general references to distribution theory mentioned in Section 1.3.2.3.1 the reader may consult the books by Zemanian (1965, 1968). Lavoine (1963) contains tables of Fourier transforms of distributions.

1.3.2.5.2. \mathcal{S} as a test-function space

A notion of convergence has to be introduced in $\mathcal{S}(\mathbb{R}^n)$ in order to be able to define and test the continuity of linear functionals on it.

A sequence (φ_j) of functions in \mathcal{S} will be said to converge to 0 if, for any given multi-indices \mathbf{k} and \mathbf{p} , the sequence $(\mathbf{x}^{\mathbf{k}} D^{\mathbf{p}} \varphi_j)$ tends to 0 uniformly on \mathbb{R}^n .

It can be shown that $\mathcal{D}(\mathbb{R}^n)$ is dense in $\mathcal{S}(\mathbb{R}^n)$. Translation is continuous for this topology. For any linear differential operator $P(D) = \sum_{\mathbf{p}} a_{\mathbf{p}} D^{\mathbf{p}}$ and any polynomial $Q(\mathbf{x})$ over \mathbb{R}^n , $(\varphi_j) \rightarrow 0$ implies $[Q(\mathbf{x}) \times P(D)\varphi_j] \rightarrow 0$ in the topology of \mathcal{S} . Therefore, differentiation and multiplication by polynomials are continuous for the topology on \mathcal{S} .

The Fourier transformations \mathcal{F} and $\tilde{\mathcal{F}}$ are also continuous for the topology of \mathcal{S} . Indeed, let (φ_j) converge to 0 for the topology on \mathcal{S} . Then, by Section 1.3.2.4.2,

$$\|(2\pi\xi)^{\mathbf{m}} D^{\mathbf{p}} (\mathcal{F}[\varphi_j])\|_{\infty} \leq \|D^{\mathbf{m}} [(2\pi\mathbf{x})^{\mathbf{p}} \varphi_j]\|_1.$$

The right-hand side tends to 0 as $j \rightarrow \infty$ by definition of convergence in \mathcal{S} , hence $\|\xi\|^{\mathbf{m}} D^{\mathbf{p}} (\mathcal{F}[\varphi_j]) \rightarrow 0$ uniformly, so that $(\mathcal{F}[\varphi_j]) \rightarrow 0$ in \mathcal{S} as $j \rightarrow \infty$. The same proof applies to $\tilde{\mathcal{F}}$.

1.3.2.5.3. Definition and examples of tempered distributions

A distribution $T \in \mathcal{D}'(\mathbb{R}^n)$ is said to be *tempered* if it can be extended into a continuous linear functional on \mathcal{S} .

If $\mathcal{S}'(\mathbb{R}^n)$ is the topological dual of $\mathcal{S}(\mathbb{R}^n)$, and if $S \in \mathcal{S}'(\mathbb{R}^n)$, then its restriction to \mathcal{D} is a tempered distribution; conversely, if $T \in \mathcal{D}'$ is tempered, then its extension to \mathcal{S} is unique (because \mathcal{D} is dense in \mathcal{S}), hence it defines an element S of \mathcal{S}' . We may therefore identify \mathcal{S}' and the space of tempered distributions.

A distribution with compact support is tempered, *i.e.* $\mathcal{S}' \supset \mathcal{E}'$. By transposition of the corresponding properties of \mathcal{S} , it is readily established that the derivative, translate or product by a polynomial of a tempered distribution is still a tempered distribution.

These inclusion relations may be summarized as follows: since \mathcal{S} contains \mathcal{D} but is contained in \mathcal{E} , the reverse inclusions hold for the topological duals, and hence \mathcal{S}' contains \mathcal{E}' but is contained in \mathcal{D}' .

A locally summable function f on \mathbb{R}^n will be said to be of *polynomial growth* if $|f(\mathbf{x})|$ can be majorized by a polynomial in $\|\mathbf{x}\|$ as $\|\mathbf{x}\| \rightarrow \infty$. It is easily shown that such a function f defines a tempered distribution T_f via

$$\langle T_f, \varphi \rangle = \int_{\mathbb{R}^n} f(\mathbf{x}) \varphi(\mathbf{x}) d^n \mathbf{x}.$$

In particular, polynomials over \mathbb{R}^n define tempered distributions, and so do functions in \mathcal{S} . The latter remark, together with the transposition identity (Section 1.3.2.4.4), invites the extension of \mathcal{F} and $\tilde{\mathcal{F}}$ from \mathcal{S} to \mathcal{S}' .

1.3.2.5.4. Fourier transforms of tempered distributions

The Fourier transform $\mathcal{F}[T]$ and cotransform $\tilde{\mathcal{F}}[T]$ of a tempered distribution T are defined by

$$\begin{aligned} \langle \mathcal{F}[T], \varphi \rangle &= \langle T, \mathcal{F}[\varphi] \rangle \\ \langle \tilde{\mathcal{F}}[T], \varphi \rangle &= \langle T, \tilde{\mathcal{F}}[\varphi] \rangle \end{aligned}$$

for all test functions $\varphi \in \mathcal{S}$. Both $\mathcal{F}[T]$ and $\tilde{\mathcal{F}}[T]$ are themselves tempered distributions, since the maps $\varphi \mapsto \mathcal{F}[\varphi]$ and $\varphi \mapsto \tilde{\mathcal{F}}[\varphi]$

are both linear and continuous for the topology of \mathcal{S} . In the same way that \mathbf{x} and ξ have been used consistently as arguments for φ and $\mathcal{F}[\varphi]$, respectively, the notation $T_{\mathbf{x}}$ and $\mathcal{F}[T]_{\xi}$ will be used to indicate which variables are involved.

When T is a distribution with compact support, its Fourier transform may be written

$$\mathcal{F}[T_{\mathbf{x}}]_{\xi} = \langle T_{\mathbf{x}}, \exp(-2\pi i \xi \cdot \mathbf{x}) \rangle$$

since the function $\mathbf{x} \mapsto \exp(-2\pi i \xi \cdot \mathbf{x})$ is in \mathcal{E} while $T_{\mathbf{x}} \in \mathcal{E}'$. It can be shown, as in Section 1.3.2.4.2, to be analytically continuable into an entire function over \mathbb{C}^n .

1.3.2.5.5. Transposition of basic properties

The duality between differentiation and multiplication by a monomial extends from \mathcal{S} to \mathcal{S}' by transposition:

$$\begin{aligned} \mathcal{F}[D_{\mathbf{x}}^{\mathbf{p}} T_{\mathbf{x}}]_{\xi} &= (2\pi i \xi)^{\mathbf{p}} \mathcal{F}[T_{\mathbf{x}}]_{\xi} \\ D_{\xi}^{\mathbf{p}} (\mathcal{F}[T_{\mathbf{x}}]_{\xi}) &= \mathcal{F}[(-2\pi i \mathbf{x})^{\mathbf{p}} T_{\mathbf{x}}]_{\xi}. \end{aligned}$$

Analogous formulae hold for $\tilde{\mathcal{F}}$, with i replaced by $-i$.

The formulae expressing the duality between translation and phase shift, *e.g.*

$$\begin{aligned} \mathcal{F}[\tau_{\mathbf{a}} T_{\mathbf{x}}]_{\xi} &= \exp(-2\pi i \mathbf{a} \cdot \xi) \mathcal{F}[T_{\mathbf{x}}]_{\xi} \\ \tau_{\alpha} (\mathcal{F}[T_{\mathbf{x}}]_{\xi}) &= \mathcal{F}[\exp(2\pi i \alpha \cdot \mathbf{x}) T_{\mathbf{x}}]_{\xi}; \end{aligned}$$

between a linear change of variable and its contragredient, *e.g.*

$$\mathcal{F}[A^{\#} T] = |\det \mathbf{A}| [(A^{-1})^T]^{\#} \mathcal{F}[T];$$

are obtained similarly by transposition from the corresponding identities in \mathcal{S} . They give a transposition formula for an affine change of variables $\mathbf{x} \mapsto S(\mathbf{x}) = \mathbf{A}\mathbf{x} + \mathbf{b}$ with non-singular matrix \mathbf{A} :

$$\begin{aligned} \mathcal{F}[S^{\#} T] &= \exp(-2\pi i \xi \cdot \mathbf{b}) \mathcal{F}[A^{\#} T] \\ &= \exp(-2\pi i \xi \cdot \mathbf{b}) |\det \mathbf{A}| [(A^{-1})^T]^{\#} \mathcal{F}[T], \end{aligned}$$

with a similar result for $\tilde{\mathcal{F}}$, replacing $-i$ by $+i$.

Conjugate symmetry is obtained similarly:

$$\mathcal{F}[\bar{T}] = \overline{\mathcal{F}[T]}, \quad \mathcal{F}[\check{T}] = \overline{\mathcal{F}[T]},$$

with the same identities for $\tilde{\mathcal{F}}$.

The tensor product property also transposes to tempered distributions: if $U \in \mathcal{S}'(\mathbb{R}^m), V \in \mathcal{S}'(\mathbb{R}^n)$,

$$\begin{aligned} \mathcal{F}[U_{\mathbf{x}} \otimes V_{\mathbf{y}}] &= \mathcal{F}[U]_{\xi} \otimes \mathcal{F}[V]_{\eta} \\ \tilde{\mathcal{F}}[U_{\mathbf{x}} \otimes V_{\mathbf{y}}] &= \tilde{\mathcal{F}}[U]_{\xi} \otimes \tilde{\mathcal{F}}[V]_{\eta}. \end{aligned}$$

1.3.2.5.6. Transforms of δ -functions

Since δ has compact support,

$$\mathcal{F}[\delta_{\mathbf{x}}]_{\xi} = \langle \delta_{\mathbf{x}}, \exp(-2\pi i \xi \cdot \mathbf{x}) \rangle = 1_{\xi}, \quad \text{i.e. } \mathcal{F}[\delta] = 1.$$

It is instructive to show that conversely $\mathcal{F}[1] = \delta$ without invoking the reciprocity theorem. Since $\partial_j 1 = 0$ for all $j = 1, \dots, n$, it follows from Section 1.3.2.3.9.4 that $\mathcal{F}[1] = c\delta$; the constant c can be determined by using the invariance of the standard Gaussian G established in Section 1.3.2.4.3:

$$\langle \mathcal{F}[1]_{\mathbf{x}}, G_{\mathbf{x}} \rangle = \langle 1_{\xi}, G_{\xi} \rangle = 1;$$

hence $c = 1$. Thus, $\mathcal{F}[1] = \delta$.

The basic properties above then read (using multi-indices to denote differentiation):