whenever the integral exists. This is the case when f and g are both in $L^1(\mathbb{R}^n)$; then $f * g$ is also in $L^1(\mathbb{R}^n)$. Let S, T and W denote the distributions associated to f, g and $f * g$, respectively: a change of variable immediately shows that for any $\varphi \in \mathscr{D}(\mathbb{R}^n)$,

$$\langle W, \varphi \rangle = \int_{\mathbb{R}^n \times \mathbb{R}^n} f(\mathbf{x}) g(\mathbf{y}) \varphi(\mathbf{x} + \mathbf{y}) \, \mathrm{d}^n\mathbf{x} \, \mathrm{d}^n\mathbf{y}.$$

Introducing the map σ from $\mathbb{R}^n \times \mathbb{R}^n$ to $\mathbb{R}^n$ defined by $\sigma(\mathbf{x}, \mathbf{y}) = \mathbf{x} + \mathbf{y}$, the latter expression may be written:

$$\langle S_{\mathbf{x}} \otimes T_{\mathbf{y}}, \varphi \circ \sigma \rangle$$

(where $\circ$ denotes the composition of mappings) or by a slight abuse of notation:

$$\langle W, \varphi \rangle = \langle S_{\mathbf{x}} \otimes T_{\mathbf{y}}, \varphi(\mathbf{x} + \mathbf{y}) \rangle.$$

A difficulty arises in extending this definition to general distributions S and T because the mapping σ is not proper: if K is compact in $\mathbb{R}^n$, then $\sigma^{-1}(K)$ is a cylinder with base K and generator the 'second bisector' $\mathbf{x} + \mathbf{y} = \mathbf{0}$ in $\mathbb{R}^n \times \mathbb{R}^n$. However, $\langle S \otimes T, \varphi \circ \sigma \rangle$ is defined whenever the intersection between Supp $(S \otimes T) =$ (Supp S) $\times$ (Supp T) and σ^{-1}(Supp φ) is compact.

We may therefore define the *convolution* $S * T$ of two distributions S and T on $\mathbb{R}^n$ by

$$\langle S * T, \varphi \rangle = \langle S \otimes T, \varphi \circ \sigma \rangle = \langle S_{\mathbf{x}} \otimes T_{\mathbf{y}}, \varphi(\mathbf{x} + \mathbf{y}) \rangle$$

whenever the following *support condition* is fulfilled:

'the set $\{(\mathbf{x}, \mathbf{y}) | \mathbf{x} \in A, \mathbf{y} \in B, \mathbf{x} + \mathbf{y} \in K\}$ is compact in $\mathbb{R}^n \times \mathbb{R}^n$ for all K compact in $\mathbb{R}^n$'.

The latter condition is met, in particular, if S or T has compact support. The support of $S * T$ is easily seen to be contained in the closure of the vector sum

$$A + B = \{\mathbf{x} + \mathbf{y} | \mathbf{x} \in A, \mathbf{y} \in B\}.$$

Convolution by a fixed distribution S is a *continuous* operation for the topology on $\mathscr{D}'$: it maps convergent sequences (T_j) to convergent sequences $(S * T_j)$. Convolution is commutative: $S * T = T * S$.

The convolution of p distributions $T_1, \ldots, T_p$ with supports $A_1, \ldots, A_p$ can be defined by

$$\langle T_1 * \ldots * T_p, \varphi \rangle = \langle (T_1)_{\mathbf{x}_1} \otimes \ldots \otimes (T_p)_{\mathbf{x}_p}, \varphi(\mathbf{x}_1 + \ldots + \mathbf{x}_p) \rangle$$

whenever the following generalized support condition:

'the set $\{(\mathbf{x}_1, \ldots, \mathbf{x}_p) | \mathbf{x}_1 \in A_1, \ldots, \mathbf{x}_p \in A_p, \mathbf{x}_1 + \ldots + \mathbf{x}_p \in K\}$ is compact in $(\mathbb{R}^n)^p$ for all K compact in $\mathbb{R}^n$'

is satisfied. It is then associative. Interesting examples of associativity failure, which can be traced back to violations of the support condition, may be found in Bracewell (1986, pp. 436–437).

It follows from previous definitions that, for all distributions $T \in \mathscr{D}'$, the following identities hold:

(i) $\delta * T = T$: δ is the unit convolution;

(ii) $\delta_{(\mathbf{a})} * T = \tau_{\mathbf{a}} T$: translation is a convolution with the corresponding translate of δ;

(iii) $(D^{\mathbf{p}}\delta) * T = D^{\mathbf{p}} T$: differentiation is a convolution with the corresponding derivative of δ;

(iv) translates or derivatives of a convolution may be obtained by translating or differentiating any one of the factors: convolution 'commutes' with translation and differentiation, a property used in Section 1.3.4.4.7.7 to speed up least-squares model refinement for macromolecules.

The latter property is frequently used for the purpose of *regularization*: if T is a distribution, α an infinitely differentiable function, and at least one of the two has compact support, then $T * \alpha$ is an infinitely differentiable ordinary function. Since sequences (α_ν) of such functions α can be constructed which have compact support and converge to δ, it follows that any distribution T can be obtained as the limit of infinitely differentiable functions $T * \alpha_\nu$. In topological jargon: $\mathscr{D}(\mathbb{R}^n)$ is 'everywhere dense' in $\mathscr{D}'(\mathbb{R}^n)$. A standard function in $\mathscr{D}$ which is often used for such proofs is defined as follows: put

$$\theta(x) = \frac{1}{A} \exp\left(-\frac{1}{1 - x^2}\right) \quad \text{for } |x| \leq 1,$$

$$= 0 \quad \text{for } |x| \geq 1,$$

with

$$A = \int_{-1}^{+1} \exp\left(-\frac{1}{1 - x^2}\right) \mathrm{d}x$$

(so that θ is in $\mathscr{D}$ and is normalized), and put

$$\theta_\varepsilon(x) = \frac{1}{\varepsilon} \theta\left(\frac{x}{\varepsilon}\right) \quad \text{in dimension 1,}$$

$$\theta_\varepsilon(\mathbf{x}) = \prod_{j=1}^{n} \theta_\varepsilon(x_j) \quad \text{in dimension } n.$$

Another related result, also proved by convolution, is the *structure theorem*: the restriction of a distribution $T \in \mathscr{D}'(\mathbb{R}^n)$ to a bounded open set Ω in $\mathbb{R}^n$ is a derivative of finite order of a continuous function.

Properties (i) to (iv) are the basis of the symbolic or operational calculus (see Carslaw & Jaeger, 1948; Van der Pol & Bremmer, 1955; Churchill, 1958; Erdélyi, 1962; Moore, 1971) for solving integro-differential equations with constant coefficients by turning them into convolution equations, then using factorization methods for convolution algebras (Schwartz, 1965).

1.3.2.4. *Fourier transforms of functions*

1.3.2.4.1. *Introduction*

Given a complex-valued function f on $\mathbb{R}^n$ subject to suitable regularity conditions, its Fourier transform $\mathscr{F}[f]$ and Fourier cotransform $\bar{\mathscr{F}}[f]$ are defined as follows:

$$\mathscr{F}[f](\xi) = \int_{\mathbb{R}^n} f(\mathbf{x}) \exp(-2\pi i \boldsymbol{\xi} \cdot \mathbf{x}) \, \mathrm{d}^n\mathbf{x}$$

$$\bar{\mathscr{F}}[f](\xi) = \int_{\mathbb{R}^n} f(\mathbf{x}) \exp(+2\pi i \boldsymbol{\xi} \cdot \mathbf{x}) \, \mathrm{d}^n\mathbf{x},$$

where $\boldsymbol{\xi} \cdot \mathbf{x} = \sum_{i=1}^{n} \xi_i x_i$ is the ordinary scalar product. The terminology and sign conventions given above are the standard ones in mathematics; those used in crystallography are slightly different (see Section 1.3.4.2.1.1). These transforms enjoy a number of remarkable properties, whose natural settings entail different regularity assumptions on f: for instance, properties relating to convolution are best treated in $L^1(\mathbb{R}^n)$, while Parseval's theorem requires the Hilbert space structure of $L^2(\mathbb{R}^n)$. After a brief review of these classical properties, the Fourier transformation will be examined in a space $\mathscr{S}(\mathbb{R}^n)$ particularly well suited to accommodating the full range of its properties, which will later serve as a space of test functions to extend the Fourier transformation to distributions.

There exists an abundant literature on the 'Fourier integral'. The books by Carslaw (1930), Wiener (1933), Titchmarsh (1948), Katznelson (1968), Sneddon (1951, 1972), and Dym & McKean (1972) are particularly recommended.

1.3.2.4.2. *Fourier transforms in L^1*

1.3.2.4.2.1. *Linearity*

Both transformations $\mathscr{F}$ and $\bar{\mathscr{F}}$ are obviously linear maps from L^1 to L^∞ when these spaces are viewed as vector spaces over the field $\mathbb{C}$ of complex numbers.

1.3.2.4.2.2. *Effect of affine coordinate transformations*

$\mathscr{F}$ and $\bar{\mathscr{F}}$ turn translations into phase shifts:

$$\mathscr{F}[\tau_{\mathbf{a}} f](\boldsymbol{\xi}) = \exp(-2\pi i \boldsymbol{\xi}\cdot\mathbf{a})\mathscr{F}[f](\boldsymbol{\xi})$$
$$\bar{\mathscr{F}}[\tau_{\mathbf{a}} f](\boldsymbol{\xi}) = \exp(+2\pi i \boldsymbol{\xi}\cdot\mathbf{a})\bar{\mathscr{F}}[f](\boldsymbol{\xi}).$$

Under a general linear change of variable $\mathbf{x} \longmapsto \mathbf{A}\mathbf{x}$ with non-singular matrix $\mathbf{A}$, the transform of $A^{\#}f$ is

$$\begin{aligned}\mathscr{F}[A^{\#}f](\boldsymbol{\xi}) &= \int_{\mathbb{R}^n} f(\mathbf{A}^{-1}\mathbf{x})\exp(-2\pi i\boldsymbol{\xi}\cdot\mathbf{x})\,\mathrm{d}^n\mathbf{x}\\ &= \int_{\mathbb{R}^n} f(\mathbf{y})\exp(-2\pi i(A^T\boldsymbol{\xi})\cdot\mathbf{y})|\det\mathbf{A}|\,\mathrm{d}^n\mathbf{y}\\ &\qquad\qquad\qquad\qquad\text{by } \mathbf{x}=\mathbf{A}\mathbf{y}\\ &= |\det\mathbf{A}|\mathscr{F}[f](\mathbf{A}^T\boldsymbol{\xi})\end{aligned}$$

i.e.

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

and similarly for $\bar{\mathscr{F}}$. The matrix $(\mathbf{A}^{-1})^T$ is called the *contragredient* of matrix $\mathbf{A}$.

Under an affine change of coordinates $\mathbf{x} \longmapsto S(\mathbf{x}) = \mathbf{A}\mathbf{x} + \mathbf{b}$ with non-singular matrix $\mathbf{A}$, the transform of $S^{\#}f$ is given by

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

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

1.3.2.4.2.3. *Conjugate symmetry*

The kernels of the Fourier transformations $\mathscr{F}$ and $\bar{\mathscr{F}}$ satisfy the following identities:

$$\exp(\pm 2\pi i\boldsymbol{\xi}\cdot\mathbf{x}) = \exp\overline{[\pm 2\pi i\boldsymbol{\xi}\cdot(-\mathbf{x})]} = \exp\overline{[\pm 2\pi i(-\boldsymbol{\xi})\cdot\mathbf{x}]}.$$

As a result the transformations $\mathscr{F}$ and $\bar{\mathscr{F}}$ themselves have the following 'conjugate symmetry' properties [where the notation $\breve{f}(\mathbf{x}) = f(-\mathbf{x})$ of Section 1.3.2.2.2 will be used]:

$$\mathscr{F}[f](\boldsymbol{\xi}) = \overline{\mathscr{F}[\bar{f}](-\boldsymbol{\xi})} = \overline{\mathscr{F}[\breve{\bar{f}}](\boldsymbol{\xi})}$$
$$\mathscr{F}[f](\boldsymbol{\xi}) = \overline{\mathscr{F}[\breve{f}](\boldsymbol{\xi})}.$$

Therefore,

(i) f real $\Leftrightarrow f = \bar{f} \Leftrightarrow \mathscr{F}[f] = \overline{\mathscr{F}[f]} \Leftrightarrow \mathscr{F}[f](\boldsymbol{\xi}) = \overline{\mathscr{F}[f](-\boldsymbol{\xi})}$: $\mathscr{F}[f]$ is said to possess *Hermitian symmetry*;

(ii) f centrosymmetric $\Leftrightarrow f = \breve{f} \Leftrightarrow \mathscr{F}[f] = \overline{\mathscr{F}[\bar{f}]}$;

(iii) f real centrosymmetric $\Leftrightarrow f = \bar{f} = \breve{f} \Leftrightarrow \mathscr{F}[f] = \overline{\mathscr{F}[f]} = \overline{\mathscr{F}[\breve{f}]} \Leftrightarrow \mathscr{F}[f]$ real centrosymmetric.

Conjugate symmetry is the basis of Friedel's law (Section 1.3.4.2.1.4) in crystallography.

1.3.2.4.2.4. *Tensor product property*

Another elementary property of $\mathscr{F}$ is its naturality with respect to tensor products. Let $u \in L^1(\mathbb{R}^m)$ and $v \in L^1(\mathbb{R}^n)$, and let $\mathscr{F}_{\mathbf{x}}, \mathscr{F}_{\mathbf{y}}, \mathscr{F}_{\mathbf{x},\mathbf{y}}$ denote the Fourier transformations in $L^1(\mathbb{R}^m), L^1(\mathbb{R}^n)$ and $L^1(\mathbb{R}^m\times\mathbb{R}^n)$, respectively. Then

$$\mathscr{F}_{\mathbf{x},\mathbf{y}}[u\otimes v] = \mathscr{F}_{\mathbf{x}}[u]\otimes\mathscr{F}_{\mathbf{y}}[v].$$

Furthermore, if $f \in L^1(\mathbb{R}^m\times\mathbb{R}^n)$, then $\mathscr{F}_{\mathbf{y}}[f] \in L^1(\mathbb{R}^m)$ as a function of $\mathbf{x}$ and $\mathscr{F}_{\mathbf{x}}[f] \in L^1(\mathbb{R}^n)$ as a function of $\mathbf{y}$, and

$$\mathscr{F}_{\mathbf{x},\mathbf{y}}[f] = \mathscr{F}_{\mathbf{x}}[\mathscr{F}_{\mathbf{y}}[f]] = \mathscr{F}_{\mathbf{y}}[\mathscr{F}_{\mathbf{x}}[f]].$$

This is easily proved by using Fubini's theorem and the fact that $(\boldsymbol{\xi},\boldsymbol{\eta})\cdot(\mathbf{x},\mathbf{y}) = \boldsymbol{\xi}\cdot\mathbf{x} + \boldsymbol{\eta}\cdot\mathbf{y}$, where $\mathbf{x},\boldsymbol{\xi}\in\mathbb{R}^m, \mathbf{y},\boldsymbol{\eta}\in\mathbb{R}^n$. This property may be written:

$$\mathscr{F}_{\mathbf{x},\mathbf{y}} = \mathscr{F}_{\mathbf{x}}\otimes\mathscr{F}_{\mathbf{y}}.$$

1.3.2.4.2.5. *Convolution property*

If f and g are summable, their convolution $f * g$ exists and is summable, and

$$\mathscr{F}[f*g](\boldsymbol{\xi}) = \int_{\mathbb{R}^n}\left[\int_{\mathbb{R}^n} f(\mathbf{y})g(\mathbf{x}-\mathbf{y})\,\mathrm{d}^n\mathbf{y}\right]\exp(-2\pi i\boldsymbol{\xi}\cdot\mathbf{x})\,\mathrm{d}^n\mathbf{x}.$$

With $\mathbf{x} = \mathbf{y} + \mathbf{z}$, so that

$$\exp(-2\pi i\boldsymbol{\xi}\cdot\mathbf{x}) = \exp(-2\pi i\boldsymbol{\xi}\cdot\mathbf{y})\exp(-2\pi i\boldsymbol{\xi}\cdot\mathbf{z}),$$

and with Fubini's theorem, rearrangement of the double integral gives:

$$\mathscr{F}[f*g] = \mathscr{F}[f]\times\mathscr{F}[g]$$

and similarly

$$\bar{\mathscr{F}}[f*g] = \bar{\mathscr{F}}[f]\times\bar{\mathscr{F}}[g].$$

Thus *the Fourier transform and cotransform turn convolution into multiplication*.

1.3.2.4.2.6. *Reciprocity property*

In general, $\mathscr{F}[f]$ and $\bar{\mathscr{F}}[f]$ are not summable, and hence cannot be further transformed; however, as they are essentially bounded, their products with the Gaussians $G_t(\xi) = \exp(-2\pi^2\|\xi\|^2 t)$ are summable for all $t > 0$, and it can be shown that

$$f = \lim_{t\to 0}\bar{\mathscr{F}}[G_t\mathscr{F}[f]] = \lim_{t\to 0}\mathscr{F}[G_t\bar{\mathscr{F}}[f]],$$

where the limit is taken in the topology of the L^1 norm $\|.\|_1$. Thus $\mathscr{F}$ and $\bar{\mathscr{F}}$ are (in a sense) mutually inverse, which justifies the common practice of calling $\bar{\mathscr{F}}$ the 'inverse Fourier transformation'.

1.3.2.4.2.7. *Riemann–Lebesgue lemma*

If $f \in L^1(\mathbb{R}^n)$, *i.e.* is summable, then $\mathscr{F}[f]$ and $\bar{\mathscr{F}}[f]$ exist and are continuous and essentially bounded:

$$\|\mathscr{F}[f]\|_\infty = \|\bar{\mathscr{F}}[f]\|_\infty \le \|f\|_1.$$

In fact one has the much stronger property, whose statement constitutes the *Riemann–Lebesgue lemma*, that $\mathscr{F}[f](\boldsymbol{\xi})$ and $\bar{\mathscr{F}}[f](\boldsymbol{\xi})$ both tend to zero as $\|\boldsymbol{\xi}\|\to\infty$.

1.3.2.4.2.8. *Differentiation*

Let us now suppose that $n = 1$ and that $f \in L^1(\mathbb{R})$ is differentiable with $f' \in L^1(\mathbb{R})$. Integration by parts yields

$$\begin{aligned}\mathscr{F}[f'](\xi) &= \int_{-\infty}^{+\infty} f'(x)\exp(-2\pi i\xi\cdot x)\,\mathrm{d}x\\ &= [f(x)\exp(-2\pi i\xi\cdot x)]_{-\infty}^{+\infty}\\ &\quad + 2\pi i\xi\int_{-\infty}^{+\infty} f(x)\exp(-2\pi i\xi\cdot x)\,\mathrm{d}x.\end{aligned}$$

Since f' is summable, f has a limit when $x\to\pm\infty$, and this limit must be 0 since f is summable. Therefore

$$\mathscr{F}[f'](\xi) = (2\pi i\xi)\mathscr{F}[f](\xi)$$

with the bound

$$\|2\pi\xi\mathscr{F}[f]\|_\infty \leq \|f'\|_1$$

so that $|\mathscr{F}[f](\xi)|$ decreases faster than $1/|\xi| \to \infty$.

This result can be easily extended to several dimensions and to any multi-index $\mathbf{m}$: if f is summable and has continuous summable partial derivatives up to order $|\mathbf{m}|$, then

$$\mathscr{F}[D^{\mathbf{m}}f](\boldsymbol{\xi}) = (2\pi i\boldsymbol{\xi})^{\mathbf{m}}\mathscr{F}[f](\boldsymbol{\xi})$$

and

$$\|(2\pi\boldsymbol{\xi})^{\mathbf{m}}\mathscr{F}[f]\|_\infty \leq \|D^{\mathbf{m}}f\|_1.$$

Similar results hold for $\bar{\mathscr{F}}$, with $2\pi i\boldsymbol{\xi}$ replaced by $-2\pi i\boldsymbol{\xi}$. Thus, the more differentiable f is, with summable derivatives, the faster $\mathscr{F}[f]$ and $\bar{\mathscr{F}}[f]$ decrease at infinity.

The property of turning differentiation into multiplication by a monomial has many important applications in crystallography, for instance differential syntheses (Sections 1.3.4.2.1.9, 1.3.4.4.7.2, 1.3.4.4.7.5) and moment-generating functions [Section 1.3.4.5.2.1(*c*)].

1.3.2.4.2.9. *Decrease at infinity*

Conversely, assume that f is summable on $\mathbb{R}^n$ and that f decreases fast enough at infinity for $\mathbf{x}^{\mathbf{m}}f$ also to be summable, for some multi-index $\mathbf{m}$. Then the integral defining $\mathscr{F}[f]$ may be subjected to the differential operator $D^{\mathbf{m}}$, still yielding a convergent integral: therefore $D^{\mathbf{m}}\mathscr{F}[f]$ exists, and

$$D^{\mathbf{m}}(\mathscr{F}[f])(\boldsymbol{\xi}) = \mathscr{F}[(-2\pi i\mathbf{x})^{\mathbf{m}}f](\boldsymbol{\xi})$$

with the bound

$$\|D^{\mathbf{m}}(\mathscr{F}[f])\|_\infty = \|(2\pi\mathbf{x})^{\mathbf{m}}f\|_1.$$

Similar results hold for $\bar{\mathscr{F}}$, with $-2\pi i\mathbf{x}$ replaced by $2\pi i\mathbf{x}$. Thus, the faster f decreases at infinity, the more $\mathscr{F}[f]$ and $\bar{\mathscr{F}}[f]$ are differentiable, with bounded derivatives. This property is the converse of that described in Section 1.3.2.4.2.8, and their combination is fundamental in the definition of the function space $\mathscr{S}$ in Section 1.3.2.4.4.1, of tempered distributions in Section 1.3.2.5, and in the extension of the Fourier transformation to them.

1.3.2.4.2.10. *The Paley–Wiener theorem*

An extreme case of the last instance occurs when f has *compact support*: then $\mathscr{F}[f]$ and $\bar{\mathscr{F}}[f]$ are so regular that they may be analytically continued from $\mathbb{R}^n$ to $\mathbb{C}^n$ where they are *entire* functions, *i.e.* have no singularities at finite distance (Paley & Wiener, 1934). This is easily seen for $\mathscr{F}[f]$: giving vector $\boldsymbol{\xi} \in \mathbb{R}^n$ a vector $\boldsymbol{\eta} \in \mathbb{R}^n$ of imaginary parts leads to

$$\begin{aligned}\mathscr{F}[f](\boldsymbol{\xi} + i\boldsymbol{\eta}) &= \int_{\mathbb{R}^n} f(\mathbf{x})\exp[-2\pi i(\boldsymbol{\xi} + i\boldsymbol{\eta})\cdot\mathbf{x}]\,\mathrm{d}^n\mathbf{x} \\ &= \mathscr{F}[\exp(2\pi\boldsymbol{\eta}\cdot\mathbf{x})f](\boldsymbol{\xi}),\end{aligned}$$

where the latter transform always exists since $\exp(2\pi\boldsymbol{\eta}\cdot\mathbf{x})f$ is summable with respect to $\mathbf{x}$ for all values of $\boldsymbol{\eta}$. This analytic continuation forms the basis of the saddlepoint method in probability theory [Section 1.3.4.5.2.1(f)] and leads to the use of maximum-entropy distributions in the statistical theory of direct phase determination [Section 1.3.4.5.2.2(*e*)].

By Liouville's theorem, an entire function in $\mathbb{C}^n$ cannot vanish identically on the complement of a compact subset of $\mathbb{R}^n$ without vanishing everywhere: therefore $\mathscr{F}[f]$ cannot have compact support if f has, and hence $\mathscr{D}(\mathbb{R}^n)$ *is not stable by Fourier transformation*.

1.3.2.4.3. *Fourier transforms in* L^2

Let f belong to $L^2(\mathbb{R}^n)$, *i.e.* be such that

$$\|f\|_2 = \left(\int_{\mathbb{R}^n} |f(\mathbf{x})|^2\,\mathrm{d}^n\mathbf{x}\right)^{1/2} < \infty.$$

1.3.2.4.3.1. *Invariance of* L^2

$\mathscr{F}[f]$ and $\bar{\mathscr{F}}[f]$ exist and are functions in L^2, *i.e.* $\mathscr{F}L^2 = L^2$, $\bar{\mathscr{F}}L^2 = L^2$.

1.3.2.4.3.2. *Reciprocity*

$\mathscr{F}[\bar{\mathscr{F}}[f]] = f$ and $\bar{\mathscr{F}}[\mathscr{F}[f]] = f$, equality being taken as 'almost everywhere' equality. This again leads to calling $\bar{\mathscr{F}}$ the 'inverse Fourier transformation' rather than the Fourier cotransformation.

1.3.2.4.3.3. *Isometry*

$\mathscr{F}$ and $\bar{\mathscr{F}}$ preserve the L^2 norm:

$\|\mathscr{F}[f]\|_2 = \|\bar{\mathscr{F}}[f]\|_2 = \|f\|_2$ (Parseval's/Plancherel's theorem).

This property, which may be written in terms of the inner product $(,)$ in $L^2(\mathbb{R}^n)$ as

$$(\mathscr{F}[f], \mathscr{F}[g]) = (\bar{\mathscr{F}}[f], \bar{\mathscr{F}}[g]) = (f, g),$$

implies that $\mathscr{F}$ and $\bar{\mathscr{F}}$ are *unitary* transformations of $L^2(\mathbb{R}^n)$ into itself, *i.e.* infinite-dimensional 'rotations'.

1.3.2.4.3.4. *Eigenspace decomposition of* L^2

Some light can be shed on the geometric structure of these rotations by the following simple considerations. Note that

$$\begin{aligned}\mathscr{F}^2[f](\mathbf{x}) &= \int_{\mathbb{R}^n} \mathscr{F}[f](\boldsymbol{\xi})\exp(-2\pi i\mathbf{x}\cdot\boldsymbol{\xi})\,\mathrm{d}^n\boldsymbol{\xi} \\ &= \bar{\mathscr{F}}[\mathscr{F}[f]](-\mathbf{x}) = f(-\mathbf{x})\end{aligned}$$

so that $\mathscr{F}^4$ (and similarly $\bar{\mathscr{F}}^4$) is the identity map. Any eigenvalue of $\mathscr{F}$ or $\bar{\mathscr{F}}$ is therefore a fourth root of unity, *i.e.* ± 1 or $\pm i$, and $L^2(\mathbb{R}^n)$ splits into an orthogonal direct sum

$$\mathbf{H}_0 \otimes \mathbf{H}_1 \otimes \mathbf{H}_2 \otimes \mathbf{H}_3,$$

where $\mathscr{F}$ (respectively $\bar{\mathscr{F}}$) acts in each subspace $\mathbf{H}_k (k = 0, 1, 2, 3)$ by multiplication by $(-i)^k$. Orthonormal bases for these subspaces can be constructed from Hermite functions (*cf.* Section 1.3.2.4.4.2) This method was used by Wiener (1933, pp. 51–71).

1.3.2.4.3.5. *The convolution theorem and the isometry property*

In L^2, the convolution theorem (when applicable) and the Parseval/Plancherel theorem are not independent. Suppose that f, g, $f \times g$ and $f * g$ are all in L^2 (without questioning whether these properties are independent). Then $f * g$ may be written in terms of the inner product in L^2 as follows:

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

i.e.

$$(f * g)(\mathbf{x}) = (\tau_{\mathbf{x}}\breve{f}, g).$$

Invoking the isometry property, we may rewrite the right-hand side as

$$\begin{aligned}(\mathscr{F}[\tau_{\mathbf{x}}\check{\bar{f}}],\mathscr{F}[g]) &= (\exp(-2\pi i\mathbf{x}\cdot\boldsymbol{\xi})\overline{\mathscr{F}[f]}_{\boldsymbol{\xi}},\mathscr{F}[g]_{\boldsymbol{\xi}})\\ &= \int_{\mathbb{R}^n}(\mathscr{F}[f]\times\mathscr{F}[g])(\mathbf{x})\\ &\quad\times\exp(+2\pi i\mathbf{x}\cdot\boldsymbol{\xi})\,\mathrm{d}^n\boldsymbol{\xi}\\ &= \bar{\mathscr{F}}[\mathscr{F}[f]\times\mathscr{F}[g]],\end{aligned}$$

so that the initial identity yields the convolution theorem.

To obtain the converse implication, note that

$$\begin{aligned}(f,g) &= \int_{\mathbb{R}^n}\overline{f(\mathbf{y})}g(\mathbf{y})\,\mathrm{d}^n\mathbf{y} = (\check{\bar{f}}*g)(\mathbf{0})\\ &= \bar{\mathscr{F}}[\mathscr{F}[\check{\bar{f}}]\times\mathscr{F}[g]](\mathbf{0})\\ &= \int_{\mathbb{R}^n}\overline{\mathscr{F}[f](\boldsymbol{\xi})}\mathscr{F}[g](\boldsymbol{\xi})\,\mathrm{d}^n\boldsymbol{\xi} = (\mathscr{F}[f],\mathscr{F}[g]),\end{aligned}$$

where conjugate symmetry (Section 1.3.2.4.2.2) has been used.

These relations have an important application in the calculation by Fourier transform methods of the derivatives used in the refinement of macromolecular structures (Section 1.3.4.4.7).

1.3.2.4.4. *Fourier transforms in $\mathscr{S}$*

1.3.2.4.4.1. *Definition and properties of $\mathscr{S}$*

The duality established in Sections 1.3.2.4.2.8 and 1.3.2.4.2.9 between the local differentiability of a function and the rate of decrease at infinity of its Fourier transform prompts one to consider the space $\mathscr{S}(\mathbb{R}^n)$ of functions f on $\mathbb{R}^n$ which are infinitely differentiable *and* all of whose derivatives are rapidly decreasing, so that for all multi-indices $\mathbf{k}$ and $\mathbf{p}$

$$(\mathbf{x}^{\mathbf{k}}D^{\mathbf{p}}f)(\mathbf{x})\to 0\quad\text{as }\|\mathbf{x}\|\to\infty.$$

The product of $f\in\mathscr{S}$ by any polynomial over $\mathbb{R}^n$ is still in $\mathscr{S}$ ($\mathscr{S}$ is an algebra over the ring of polynomials). Furthermore, $\mathscr{S}$ is invariant under translations and differentiation.

If $f\in\mathscr{S}$, then its transforms $\mathscr{F}[f]$ and $\bar{\mathscr{F}}[f]$ are

(i) infinitely differentiable because f is rapidly decreasing;

(ii) rapidly decreasing because f is infinitely differentiable;

hence $\mathscr{F}[f]$ and $\bar{\mathscr{F}}[f]$ are in $\mathscr{S}$: *$\mathscr{S}$ is invariant* under $\mathscr{F}$ and $\bar{\mathscr{F}}$.

Since $L^1\supset\mathscr{S}$ and $L^2\supset\mathscr{S}$, all properties of $\mathscr{F}$ and $\bar{\mathscr{F}}$ already encountered above are enjoyed by functions of $\mathscr{S}$, with all restrictions on differentiability and/or integrability lifted. For instance, given two functions f and g in $\mathscr{S}$, then both fg and $f*g$ are in $\mathscr{S}$ (which was not the case with L^1 nor with L^2) so that the reciprocity theorem inherited from L^2

$$\mathscr{F}[\bar{\mathscr{F}}[f]]=f\quad\text{and}\quad\bar{\mathscr{F}}[\mathscr{F}[f]]=f$$

allows one to state the reverse of the convolution theorem first established in L^1:

$$\begin{aligned}\mathscr{F}[fg] &= \mathscr{F}[f]*\mathscr{F}[g]\\ \bar{\mathscr{F}}[fg] &= \bar{\mathscr{F}}[f]*\bar{\mathscr{F}}[g].\end{aligned}$$

1.3.2.4.4.2. *Gaussian functions and Hermite functions*

Gaussian functions are particularly important elements of $\mathscr{S}$. In dimension 1, a well known contour integration (Schwartz, 1965, p. 184) yields

$$\mathscr{F}[\exp(-\pi x^2)](\xi)=\bar{\mathscr{F}}[\exp(-\pi x^2)](\xi)=\exp(-\pi\xi^2),$$

which shows that the 'standard Gaussian' $\exp(-\pi x^2)$ is invariant under $\mathscr{F}$ and $\bar{\mathscr{F}}$. By a tensor product construction, it follows that the same is true of the standard Gaussian

$$G(\mathbf{x})=\exp(-\pi\|\mathbf{x}\|^2)$$

in dimension n:

$$\mathscr{F}[G](\boldsymbol{\xi})=\bar{\mathscr{F}}[G](\boldsymbol{\xi})=G(\boldsymbol{\xi}).$$

In other words, G is an eigenfunction of $\mathscr{F}$ and $\bar{\mathscr{F}}$ for eigenvalue 1 (Section 1.3.2.4.3.4).

A complete system of eigenfunctions may be constructed as follows. In dimension 1, consider the family of functions

$$H_m=\frac{D^mG^2}{G}\quad(m\geq 0),$$

where D denotes the differentiation operator. The first two members of the family

$$H_0=G,\qquad H_1=2DG,$$

are such that $\mathscr{F}[H_0]=H_0$, as shown above, and

$$DG(x)=-2\pi xG(x)=i(2\pi ix)G(x)=i\mathscr{F}[DG](x),$$

hence

$$\mathscr{F}[H_1]=(-i)H_1.$$

We may thus take as an induction hypothesis that

$$\mathscr{F}[H_m]=(-i)^mH_m.$$

The identity

$$D\left(\frac{D^mG^2}{G}\right)=\frac{D^{m+1}G^2}{G}-\frac{DG}{G}\frac{D^mG^2}{G}$$

may be written

$$H_{m+1}(x)=(DH_m)(x)-2\pi xH_m(x),$$

and the two differentiation theorems give:

$$\begin{aligned}\mathscr{F}[DH_m](\xi) &= (2\pi i\xi)\mathscr{F}[H_m](\xi)\\ \mathscr{F}[-2\pi xH_m](\xi) &= -iD(\mathscr{F}[H_m])(\xi).\end{aligned}$$

Combination of this with the induction hypothesis yields

$$\begin{aligned}\mathscr{F}[H_{m+1}](\xi) &= (-i)^{m+1}[(DH_m)(\xi)-2\pi\xi H_m(\xi)]\\ &= (-i)^{m+1}H_{m+1}(\xi),\end{aligned}$$

thus proving that H_m is an eigenfunction of $\mathscr{F}$ for eigenvalue $(-i)^m$ for all $m\geq 0$. The same proof holds for $\bar{\mathscr{F}}$, with eigenvalue i^m. If these eigenfunctions are normalized as

$$\mathscr{H}_m(x)=\frac{(-1)^m2^{1/4}}{\sqrt{m!}2^m\pi^{m/2}}H_m(x),$$

then it can be shown that the collection of *Hermite functions* $\{\mathscr{H}_m(x)\}_{m\geq 0}$ constitutes an orthonormal basis of $L^2(\mathbb{R})$ such that $\mathscr{H}_m$ is an eigenfunction of $\mathscr{F}$ (respectively $\bar{\mathscr{F}}$) for eigenvalue $(-i)^m$ (respectively i^m).

In dimension n, the same construction can be extended by tensor product to yield the multivariate Hermite functions

$$\mathscr{H}_{\mathbf{m}}(\mathbf{x})=\mathscr{H}_{m_1}(x_1)\times\mathscr{H}_{m_2}(x_2)\times\ldots\times\mathscr{H}_{m_n}(x_n)$$

(where $\mathbf{m}\geq\mathbf{0}$ is a multi-index). These constitute an orthonormal basis of $L^2(\mathbb{R}^n)$, with $\mathscr{H}_{\mathbf{m}}$ an eigenfunction of $\mathscr{F}$ (respectively $\bar{\mathscr{F}}$) for eigenvalue $(-i)^{|\mathbf{m}|}$ (respectively $i^{|\mathbf{m}|}$). Thus the subspaces $\mathbf{H}_k$ of Section 1.3.2.4.3.4 are spanned by those $\mathscr{H}_{\mathbf{m}}$ with $|\mathbf{m}|\equiv k \bmod 4$ $(k=0,1,2,3)$.

General multivariate Gaussians are usually encountered in the non-standard form

$$G_{\mathbf{A}}(\mathbf{x})=\exp(-\tfrac{1}{2}\mathbf{x}^T\cdot\mathbf{A}\mathbf{x}),$$

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

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

i.e.

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

i.e. finally

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

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 $\bar{\mathscr{F}}$, shows that the 'peakier' $G_{\mathbf{A}}$, the 'broader' $\mathscr{F}[G_{\mathbf{A}}]$. This is a general property of the Fourier transformation, expressed in dimension 1 by the *Heisenberg inequality* (Weyl, 1931):

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

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 $\mathscr{F}[f]$ behave at infinity as constant multiples of G, then each of them is *everywhere* a constant multiple of G; if both f and $\mathscr{F}[f]$ 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 $\mathscr{F}[f]$ 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 $\mathscr{S}$, is its *symmetry*: if f and g are in $\mathscr{S}$, then by Fubini's theorem

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

This possibility of 'transposing' $\mathscr{F}$ (and $\bar{\mathscr{F}}$) 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

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

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

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

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 $\mathscr{F}$ and $\bar{\mathscr{F}}$.

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 $\mathscr{D}$ is not invariant under $\mathscr{F}$ and $\bar{\mathscr{F}}$. By contrast, the space $\mathscr{S}$ of infinitely differentiable rapidly decreasing functions *is* invariant under $\mathscr{F}$ and $\bar{\mathscr{F}}$, and furthermore transposition formulae such as

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

hold for all $f, g \in \mathscr{S}$. 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 $\mathscr{S}$ instead of $\mathscr{D}$ as a space of test functions φ, and defining the Fourier transform $\mathscr{F}[T]$ of a distribution T by

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

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