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

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

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

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

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

hence

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

We may thus take as an induction hypothesis that

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

The identity

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

may be written

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

and the two differentiation theorems give:

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

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

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

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.