International Tables for Crystallography (2006). Vol. B, Section 1.3.2.4.2, pp. 35–37.

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]:

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

Therefore,

(i) f real $\Leftrightarrow f = \bar{f} \Leftrightarrow \mathscr{F}[f] = \overline{\breve{\mathscr{F}[f]}} \Leftrightarrow \mathscr{F}[f](\boldsymbol{\xi}) = \overline{\mathscr{F}[f](-\boldsymbol{\xi})}$: $\mathscr{F}[f]$ 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 $\Leftrightarrow f = \bar{f} = \breve{f} \Leftrightarrow \mathscr{F}[f] = \overline{\mathscr{F}[f]} = \overline{\breve{\mathscr{F}[f]}} \Leftrightarrow \mathscr{F}[f]$ 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:

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

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.

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

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

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

so that the initial identity yields the convolution theorem.

To obtain the converse implication, note that

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

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 **k** and **p**

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

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:

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

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

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

references