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

so that the initial identity yields the convolution theorem.

To obtain the converse implication, note that

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

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 $\mathcal{S}$*

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

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 $\mathcal{S}(\mathbb{R}^n)$ 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**

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

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

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

(i) infinitely differentiable because f is rapidly decreasing;

(ii) rapidly decreasing because f is infinitely differentiable;

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

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

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

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

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

1.3.2.4.4.2. *Gaussian functions and Hermite functions*

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

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

which shows that the 'standard Gaussian' $\exp(-\pi x^2)$ is invariant under $\mathcal{F}$ and $\bar{\mathcal{F}}$. 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:

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

In other words, G is an eigenfunction of $\mathcal{F}$ and $\bar{\mathcal{F}}$ 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 $\mathcal{F}[H_0] = H_0$, as shown above, and

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

hence

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

We may thus take as an induction hypothesis that

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

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:

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

Combination of this with the induction hypothesis yields

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

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

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

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

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

(where $\mathbf{m} \geq \mathbf{0}$ is a multi-index). These constitute an orthonormal basis of $L^2(\mathbb{R}^n)$, with $\mathcal{H}_{\mathbf{m}}$ an eigenfunction of $\mathcal{F}$ (respectively $\bar{\mathcal{F}}$) 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 $\mathcal{H}_{\mathbf{m}}$ with $|\mathbf{m}| \equiv k \bmod 4$ $(k = 0, 1, 2, 3)$.

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

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