International Tables for Crystallography (2006). Vol. B, Section 1.3.2.4.4.4, p. 38.

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

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

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 $\bar{\mathcal{F}}$, 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):

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

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 $\mathcal{F}[f]$ 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

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

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

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

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

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

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

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 $\bar{\mathcal{F}}$. By contrast, the space $\mathcal{S}$ of infinitely differentiable rapidly decreasing functions *is* invariant under $\mathcal{F}$ and $\bar{\mathcal{F}}$, 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 $\mathcal{D}'$, 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.