International Tables for Crystallography (2006). Vol. B, Section 1.3.2.4.2.8, pp. 35–36.

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:

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

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

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

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]:

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

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:

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

i.e.

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

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

references