International Tables for Crystallography (2006). Vol. B, Section 1.3.2.4.2.1, p. 35.

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

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

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]:

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

Therefore,

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

references