

1.3. FOURIER TRANSFORMS IN CRYSTALLOGRAPHY

1.3.2.4.2. Fourier transforms in  $L^1$

1.3.2.4.2.1. Linearity

Both transformations  $\mathcal{F}$  and  $\tilde{\mathcal{F}}$  are obviously linear maps from  $L^1$  to  $L^\infty$  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

$\mathcal{F}$  and  $\tilde{\mathcal{F}}$  turn translations into phase shifts:

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

Under a general linear change of variable  $\mathbf{x} \mapsto \mathbf{A}\mathbf{x}$  with non-singular matrix  $\mathbf{A}$ , the transform of  $A^\#f$  is

$$\begin{aligned} \mathcal{F}[A^\#f](\boldsymbol{\xi}) &= \int_{\mathbb{R}^n} f(\mathbf{A}^{-1}\mathbf{x}) \exp(-2\pi i \boldsymbol{\xi} \cdot \mathbf{x}) d^n \mathbf{x} \\ &= \int_{\mathbb{R}^n} f(\mathbf{y}) \exp(-2\pi i (\mathbf{A}^T \boldsymbol{\xi}) \cdot \mathbf{y}) |\det \mathbf{A}| d^n \mathbf{y} \\ & \hspace{15em} \text{by } \mathbf{x} = \mathbf{A}\mathbf{y} \\ &= |\det \mathbf{A}| \mathcal{F}[f](\mathbf{A}^T \boldsymbol{\xi}) \end{aligned}$$

i.e.

$$\mathcal{F}[A^\#f] = |\det \mathbf{A}| [(\mathbf{A}^{-1})^T]^\# \mathcal{F}[f]$$

and similarly for  $\tilde{\mathcal{F}}$ . The matrix  $(\mathbf{A}^{-1})^T$  is called the *contragredient* of matrix  $\mathbf{A}$ .

Under an affine change of coordinates  $\mathbf{x} \mapsto S(\mathbf{x}) = \mathbf{A}\mathbf{x} + \mathbf{b}$  with non-singular matrix  $\mathbf{A}$ , the transform of  $S^\#f$  is given by

$$\begin{aligned} \mathcal{F}[S^\#f](\boldsymbol{\xi}) &= \mathcal{F}[\tau_{\mathbf{b}}(A^\#f)](\boldsymbol{\xi}) \\ &= \exp(-2\pi i \boldsymbol{\xi} \cdot \mathbf{b}) \mathcal{F}[A^\#f](\boldsymbol{\xi}) \\ &= \exp(-2\pi i \boldsymbol{\xi} \cdot \mathbf{b}) |\det \mathbf{A}| \mathcal{F}[f](\mathbf{A}^T \boldsymbol{\xi}) \end{aligned}$$

with a similar result for  $\tilde{\mathcal{F}}$ , replacing  $-i$  by  $+i$ .

1.3.2.4.2.3. Conjugate symmetry

The kernels of the Fourier transformations  $\mathcal{F}$  and  $\tilde{\mathcal{F}}$  satisfy the following identities:

$$\exp(\pm 2\pi i \boldsymbol{\xi} \cdot \mathbf{x}) = \exp[\pm 2\pi i \boldsymbol{\xi} \cdot (-\mathbf{x})] = \exp[\pm 2\pi i (-\boldsymbol{\xi}) \cdot \mathbf{x}].$$

As a result the transformations  $\mathcal{F}$  and  $\tilde{\mathcal{F}}$  themselves have the following ‘conjugate symmetry’ properties [where the notation  $\check{f}(\mathbf{x}) = f(-\mathbf{x})$  of Section 1.3.2.2.2 will be used]:

$$\begin{aligned} \mathcal{F}[f](\boldsymbol{\xi}) &= \overline{\mathcal{F}[\check{f}](-\boldsymbol{\xi})} = \overline{\mathcal{F}[\check{f}]}(\boldsymbol{\xi}) \\ \tilde{\mathcal{F}}[f](\boldsymbol{\xi}) &= \tilde{\mathcal{F}}[\check{f}](\boldsymbol{\xi}). \end{aligned}$$

Therefore,

- (i)  $f$  real  $\Leftrightarrow f = \bar{f} \Leftrightarrow \mathcal{F}[f] = \overline{\mathcal{F}[\check{f}]} \Leftrightarrow \mathcal{F}[f](\boldsymbol{\xi}) = \overline{\mathcal{F}[f](-\boldsymbol{\xi})}$ :  $\mathcal{F}[f]$  is said to possess *Hermitian symmetry*;
- (ii)  $f$  centrosymmetric  $\Leftrightarrow f = \check{f} \Leftrightarrow \mathcal{F}[f] = \mathcal{F}[\check{f}]$ ;
- (iii)  $f$  real centrosymmetric  $\Leftrightarrow f = \bar{f} = \check{f} \Leftrightarrow \mathcal{F}[f] = \overline{\mathcal{F}[\check{f}]} = \overline{\mathcal{F}[f]} \Leftrightarrow \mathcal{F}[f]$  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  $\mathcal{F}$  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  $\mathcal{F}_{\mathbf{x}}, \mathcal{F}_{\mathbf{y}}, \mathcal{F}_{\mathbf{x}, \mathbf{y}}$  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

$$\mathcal{F}_{\mathbf{x}, \mathbf{y}}[u \otimes v] = \mathcal{F}_{\mathbf{x}}[u] \otimes \mathcal{F}_{\mathbf{y}}[v].$$

Furthermore, if  $f \in L^1(\mathbb{R}^m \times \mathbb{R}^n)$ , then  $\mathcal{F}_{\mathbf{y}}[f] \in L^1(\mathbb{R}^n)$  as a function of  $\mathbf{x}$  and  $\mathcal{F}_{\mathbf{x}}[f] \in L^1(\mathbb{R}^m)$  as a function of  $\mathbf{y}$ , and

$$\mathcal{F}_{\mathbf{x}, \mathbf{y}}[f] = \mathcal{F}_{\mathbf{x}}[\mathcal{F}_{\mathbf{y}}[f]] = \mathcal{F}_{\mathbf{y}}[\mathcal{F}_{\mathbf{x}}[f]].$$

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:

$$\mathcal{F}_{\mathbf{x}, \mathbf{y}} = \mathcal{F}_{\mathbf{x}} \otimes \mathcal{F}_{\mathbf{y}}.$$

1.3.2.4.2.5. Convolution property

If  $f$  and  $g$  are summable, their convolution  $f * g$  exists and is summable, and

$$\mathcal{F}[f * g](\boldsymbol{\xi}) = \int_{\mathbb{R}^n} \left[ \int_{\mathbb{R}^n} f(\mathbf{y}) g(\mathbf{x} - \mathbf{y}) d^n \mathbf{y} \right] \exp(-2\pi i \boldsymbol{\xi} \cdot \mathbf{x}) d^n \mathbf{x}.$$

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:

$$\mathcal{F}[f * g] = \mathcal{F}[f] \times \mathcal{F}[g]$$

and similarly

$$\tilde{\mathcal{F}}[f * g] = \tilde{\mathcal{F}}[f] \times \tilde{\mathcal{F}}[g].$$

Thus the Fourier transform and cotransform turn convolution into multiplication.

1.3.2.4.2.6. Reciprocity property

In general,  $\mathcal{F}[f]$  and  $\tilde{\mathcal{F}}[f]$  are not summable, and hence cannot be further transformed; however, as they are essentially bounded, their products with the Gaussians  $G_t(\boldsymbol{\xi}) = \exp(-2\pi^2 \|\boldsymbol{\xi}\|^2 t)$  are summable for all  $t > 0$ , and it can be shown that

$$f = \lim_{t \rightarrow 0} \tilde{\mathcal{F}}[G_t \mathcal{F}[f]] = \lim_{t \rightarrow 0} \mathcal{F}[G_t \tilde{\mathcal{F}}[f]],$$

where the limit is taken in the topology of the  $L^1$  norm  $\|\cdot\|_1$ . Thus  $\tilde{\mathcal{F}}$  and  $\mathcal{F}$  are (in a sense) mutually inverse, which justifies the common practice of calling  $\tilde{\mathcal{F}}$  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  $\mathcal{F}[f]$  and  $\tilde{\mathcal{F}}[f]$  exist and are continuous and essentially bounded:

$$\|\mathcal{F}[f]\|_\infty = \|\tilde{\mathcal{F}}[f]\|_\infty \leq \|f\|_1.$$

In fact one has the much stronger property, whose statement constitutes the *Riemann–Lebesgue lemma*, that  $\mathcal{F}[f](\boldsymbol{\xi})$  and  $\tilde{\mathcal{F}}[f](\boldsymbol{\xi})$  both tend to zero as  $\|\boldsymbol{\xi}\| \rightarrow \infty$ .

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

$$\begin{aligned} \mathcal{F}[f'](\boldsymbol{\xi}) &= \int_{-\infty}^{+\infty} f'(x) \exp(-2\pi i \boldsymbol{\xi} \cdot x) dx \\ &= [f(x) \exp(-2\pi i \boldsymbol{\xi} \cdot x)]_{-\infty}^{+\infty} \\ &\quad + 2\pi i \boldsymbol{\xi} \int_{-\infty}^{+\infty} f(x) \exp(-2\pi i \boldsymbol{\xi} \cdot x) dx. \end{aligned}$$

Since  $f'$  is summable,  $f$  has a limit when  $x \rightarrow \pm\infty$ , and this limit must be 0 since  $f$  is summable. Therefore