

1.3. FOURIER TRANSFORMS IN CRYSTALLOGRAPHY

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 $\mathcal{F}[f]$ cannot have compact support if f has, and hence $\mathcal{D}(\mathbb{R}^n)$ 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

$$\|f\|_2 = \left(\int_{\mathbb{R}^n} |f(\mathbf{x})|^2 d^n \mathbf{x} \right)^{1/2} < \infty.$$

1.3.2.4.3.1. Invariance of L^2

$\mathcal{F}[f]$ and $\bar{\mathcal{F}}[f]$ exist and are functions in L^2 , i.e. $\mathcal{F}L^2 = L^2$, $\bar{\mathcal{F}}L^2 = L^2$.

1.3.2.4.3.2. Reciprocity

$\mathcal{F}[\bar{\mathcal{F}}[f]] = f$ and $\bar{\mathcal{F}}[\mathcal{F}[f]] = f$, equality being taken as 'almost everywhere' equality. This again leads to calling $\bar{\mathcal{F}}$ the 'inverse Fourier transformation' rather than the Fourier cotransformation.

1.3.2.4.3.3. Isometry

\mathcal{F} and $\bar{\mathcal{F}}$ preserve the L^2 norm:

$$\|\mathcal{F}[f]\|_2 = \|\bar{\mathcal{F}}[f]\|_2 = \|f\|_2 \text{ (Parseval's/Plancherel's theorem).}$$

This property, which may be written in terms of the inner product (\cdot, \cdot) in $L^2(\mathbb{R}^n)$ as

$$(\mathcal{F}[f], \mathcal{F}[g]) = (\bar{\mathcal{F}}[f], \bar{\mathcal{F}}[g]) = (f, g),$$

implies that \mathcal{F} and $\bar{\mathcal{F}}$ 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

$$\begin{aligned} \mathcal{F}^2[f](\mathbf{x}) &= \int_{\mathbb{R}^n} \mathcal{F}[f](\xi) \exp(-2\pi i \mathbf{x} \cdot \xi) d^n \xi \\ &= \bar{\mathcal{F}}[\bar{\mathcal{F}}[f]](-\mathbf{x}) = f(-\mathbf{x}) \end{aligned}$$

so that \mathcal{F}^4 (and similarly $\bar{\mathcal{F}}^4$) is the identity map. Any eigenvalue of \mathcal{F} or $\bar{\mathcal{F}}$ 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 \mathcal{F} (respectively $\bar{\mathcal{F}}$) 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:

$$(f * g)(\mathbf{x}) = \int_{\mathbb{R}^n} f(\mathbf{x} - \mathbf{y})g(\mathbf{y}) d^n \mathbf{y} = \int_{\mathbb{R}^n} \overline{\mathcal{F}[f(\mathbf{y} - \mathbf{x})]}g(\mathbf{y}) d^n \mathbf{y},$$

i.e.

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

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

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

so that the initial identity yields the convolution theorem.

To obtain the converse implication, note that

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

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 \mathbf{k} and \mathbf{p}

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

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

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

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