

1.3. FOURIER TRANSFORMS IN CRYSTALLOGRAPHY

The Poisson kernel

$$P_r(x) = 1 + 2 \sum_{m=1}^{\infty} r^m \cos 2\pi mx$$

$$= \frac{1 - r^2}{1 - 2r \cos 2\pi mx + r^2}$$

with $0 \leq r < 1$ gives rise to an Abel summation procedure [Tolstov (1962, p. 162); Whittaker & Watson (1927, p. 57)] since

$$(P_r * f)(x) = \sum_{m \in \mathbb{Z}} c_m(f) r^{|m|} \exp(2\pi imx).$$

Compared with the other kernels, P_r has the disadvantage of not being a trigonometric polynomial; however, P_r is the real part of the Cauchy kernel (Cartan, 1961; Ahlfors, 1966):

$$P_r(x) = \Re \left[\frac{1 + r \exp(2\pi ix)}{1 - r \exp(2\pi ix)} \right]$$

and hence provides a link between trigonometric series and analytic functions of a complex variable.

Other methods of summation involve forming a moving average of f by convolution with other sequences of functions $\alpha_p(\mathbf{x})$ besides D_p of F_p which ‘tend towards δ ’ as $p \rightarrow \infty$. The convolution is performed by multiplying the Fourier coefficients of f by those of α_p , so that one forms the quantities

$$S'_p(f)(x) = \sum_{|m| \leq p} c_m(\alpha_p) c_m(f) \exp(2\pi imx).$$

For instance the ‘sigma factors’ of Lanczos (Lanczos, 1966, p. 65), defined by

$$\sigma_m = \frac{\sin[m\pi/p]}{m\pi/p},$$

lead to a summation procedure whose behaviour is intermediate between those using the Dirichlet and the Fejér kernels; it corresponds to forming a moving average of f by convolution with

$$\alpha_p = P\chi_{[-1/(2p), 1/(2p)]} * D_p,$$

which is itself the convolution of a ‘rectangular pulse’ of width $1/p$ and of the Dirichlet kernel of order p .

A review of the summation problem in crystallography is given in Section 1.3.4.2.1.3.

1.3.2.6.10.2. Classical L^2 theory

The space $L^2(\mathbb{R}/\mathbb{Z})$ of (equivalence classes of) square-integrable complex-valued functions f on the circle is contained in $L^1(\mathbb{R}/\mathbb{Z})$, since by the Cauchy–Schwarz inequality

$$\|f\|_1^2 = \left(\int_0^1 |f(x)| \times 1 \, dx \right)^2$$

$$\leq \left(\int_0^1 |f(x)|^2 \, dx \right) \left(\int_0^1 1^2 \, dx \right) = \|f\|_2^2 \leq \infty.$$

Thus all the results derived for L^1 hold for L^2 , a great simplification over the situation in \mathbb{R} or \mathbb{R}^n where neither L^1 nor L^2 was contained in the other.

However, more can be proved in L^2 , because L^2 is a Hilbert space (Section 1.3.2.2.4) for the inner product

$$(f, g) = \int_0^1 \overline{f(x)} g(x) \, dx,$$

and because the family of functions $\{\exp(2\pi imx)\}_{m \in \mathbb{Z}}$ constitutes an orthonormal Hilbert basis for L^2 .

The sequence of Fourier coefficients $c_m(f)$ of $f \in L^2$ belongs to the space $\ell^2(\mathbb{Z})$ of square-summable sequences:

$$\sum_{m \in \mathbb{Z}} |c_m(f)|^2 < \infty.$$

Conversely, every element $c = (c_m)$ of ℓ^2 is the sequence of Fourier coefficients of a unique function in L^2 . The inner product

$$(c, d) = \sum_{m \in \mathbb{Z}} \overline{c_m} d_m$$

makes ℓ^2 into a Hilbert space, and the map from L^2 to ℓ^2 established by the Fourier transformation is an isometry (Parseval/Plancherel):

$$\|f\|_{L^2} = \|c(f)\|_{\ell^2}$$

or equivalently:

$$(f, g) = (c(f), c(g)).$$

This is a useful property in applications, since (f, g) may be calculated either from f and g themselves, or from their Fourier coefficients $c(f)$ and $c(g)$ (see Section 1.3.4.4.6) for crystallographic applications).

By virtue of the orthogonality of the basis $\{\exp(2\pi imx)\}_{m \in \mathbb{Z}}$, the partial sum $S_p(f)$ is the best mean-square fit to f in the linear subspace of L^2 spanned by $\{\exp(2\pi imx)\}_{|m| \leq p}$, and hence (Bessel’s inequality)

$$\sum_{|m| \leq p} |c_m(f)|^2 = \|f\|_2^2 - \sum_{|M| \geq p} |c_M(f)|^2 \leq \|f\|_2^2.$$

1.3.2.6.10.3. The viewpoint of distribution theory

The use of distributions enlarges considerably the range of behaviour which can be accommodated in a Fourier series, even in the case of general dimension n where classical theories meet with even more difficulties than in dimension 1.

Let $\{w_m\}_{m \in \mathbb{Z}}$ be a sequence of complex numbers with $|w_m|$ growing at most polynomially as $|m| \rightarrow \infty$, say $|w_m| \leq C|m|^K$. Then the sequence $\{w_m/(2\pi im)^{K+2}\}_{m \in \mathbb{Z}}$ is in ℓ^2 and even defines a continuous function $f \in L^2(\mathbb{R}/\mathbb{Z})$ and an associated tempered distribution $T_f \in \mathcal{D}'(\mathbb{R}/\mathbb{Z})$. Differentiation of T_f ($K+2$) times then yields a tempered distribution whose Fourier transform leads to the original sequence of coefficients. Conversely, by the structure theorem for distributions with compact support (Section 1.3.2.3.9.7), the motif T^0 of a \mathbb{Z} -periodic distribution is a derivative of finite order of a continuous function; hence its Fourier coefficients will grow at most polynomially with $|m|$ as $|m| \rightarrow \infty$.

Thus distribution theory allows the manipulation of Fourier series whose coefficients exhibit polynomial growth as their order goes to infinity, while those derived from functions had to tend to 0 by virtue of the Riemann–Lebesgue lemma. The distribution-theoretic approach to Fourier series holds even in the case of general dimension n , where classical theories meet with even more difficulties (see Ash, 1976) than in dimension 1.

1.3.2.7. The discrete Fourier transformation

1.3.2.7.1. Shannon’s sampling theorem and interpolation formula

Let $\varphi \in \mathcal{E}(\mathbb{R}^n)$ be such that $\Phi = \mathcal{F}[\varphi]$ has compact support K . Let φ be sampled at the nodes of a lattice Λ^* , yielding the lattice distribution $R^* \times \varphi$. The Fourier transform of this sampled version of φ is

$$\mathcal{F}[R^* \times \varphi] = |\det \mathbf{A}| (R * \Phi),$$