International Tables for Crystallography (2006). Vol. B, Section 1.3.2.6.10.1, pp. 44–45.

We may now state an important theorem of Szegö (1915, 1920). Let $f \in L^1$, and put $m = \text{ess inf } f$, $M = \text{ess sup } f$. If m and M are finite, then for any continuous function $F(\lambda)$ defined in the interval $[m, M]$ we have

$$\lim_{n\to\infty} \frac{1}{n+1} \sum_{\nu=1}^{n+1} F(\lambda_\nu^{(n)}) = \int_0^1 F[f(x)] \, \mathrm{d}x.$$

In other words, the eigenvalues $\lambda_\nu^{(n)}$ of the T_n and the values $f[\nu/(n+2)]$ of f on a regular subdivision of]0, 1[are equally distributed.

Further investigations into the spectra of Toeplitz matrices may be found in papers by Hartman & Wintner (1950, 1954), Kac *et al.* (1953), Widom (1965), and in the notes by Hirschman & Hughes (1977).

1.3.2.6.9.4. *Consequences of Szegö's theorem*

(i) If the λ's are ordered in ascending order, then

$$\lim_{n\to\infty} \lambda_1^{(n)} = m = \text{ess inf } f, \quad \lim_{n\to\infty} \lambda_{n+1}^{(n)} = M = \text{ess sup } f.$$

Thus, when $f \geq 0$, the condition number $\lambda_{n+1}^{(n)}/\lambda_1^{(n)}$ of $T_n[f]$ tends towards the 'essential dynamic range' M/m of f.

(ii) Let $F(\lambda) = \lambda^s$ where s is a positive integer. Then

$$\lim_{n\to\infty} \frac{1}{n+1} \sum_{\nu=1}^{n+1} [\lambda_\nu^{(n)}]^s = \int_0^1 [f(x)]^s \, \mathrm{d}x.$$

(iii) Let $m > 0$, so that $\lambda_\nu^{(n)} > 0$, and let $D_n(f) = \det T_n(f)$. Then

$$D_n(f) = \prod_{\nu=1}^{n+1} \lambda_\nu^{(n)},$$

hence

$$\log D_n(f) = \sum_{\nu=1}^{n+1} \log \lambda_\nu^{(n)}.$$

Putting $F(\lambda) = \log \lambda$, it follows that

$$\lim_{n\to\infty} [D_n(f)]^{1/(n+1)} = \exp\left\{\int_0^1 \log f(x) \, \mathrm{d}x\right\}.$$

Further terms in this limit were obtained by Szegö (1952) and interpreted in probabilistic terms by Kac (1954).

1.3.2.6.10. *Convergence of Fourier series*

The investigation of the convergence of Fourier series and of more general trigonometric series has been the subject of intense study for over 150 years [see *e.g.* Zygmund (1976)]. It has been a constant source of new mathematical ideas and theories, being directly responsible for the birth of such fields as set theory, topology and functional analysis.

This section will briefly survey those aspects of the classical results in dimension 1 which are relevant to the practical use of Fourier series in crystallography. The books by Zygmund (1959), Tolstov (1962) and Katznelson (1968) are standard references in the field, and Dym & McKean (1972) is recommended as a stimulant.

1.3.2.6.10.1. *Classical L^1 theory*

The space $L^1(\mathbb{R}/\mathbb{Z})$ consists of (equivalence classes of) complex-valued functions f on the circle which are summable, *i.e.* for which

$$\|f\|_1 \equiv \int_0^1 |f(x)| \, \mathrm{d}x < +\infty.$$

It is a convolution algebra: If f and g are in L^1, then $f * g$ is in L^1.

The mth Fourier coefficient $c_m(f)$ of f,

$$c_m(f) = \int_0^1 f(x) \exp(-2\pi i m x) \, \mathrm{d}x$$

is bounded: $|c_m(f)| \leq \|f\|_1$, and by the Riemann–Lebesgue lemma $c_m(f) \to 0$ as $m \to \infty$. By the convolution theorem, $c_m(f * g) = c_m(f) c_m(g)$.

The pth *partial sum* $S_p(f)$ of the Fourier series of f,

$$S_p(f)(x) = \sum_{|m| \leq p} c_m(f) \exp(2\pi i m x),$$

may be written, by virtue of the convolution theorem, as $S_p(f) = D_p * f$, where

$$D_p(x) = \sum_{|m| \leq p} \exp(2\pi i m x) = \frac{\sin[(2p+1)\pi x]}{\sin \pi x}$$

is the *Dirichlet kernel*. Because D_p comprises numerous slowly decaying oscillations, both positive and negative, $S_p(f)$ may not converge towards f in a strong sense as $p \to \infty$. Indeed, spectacular pathologies are known to exist where the partial sums, examined pointwise, diverge everywhere (Zygmund, 1959, Chapter VIII). When f is piecewise continuous, but presents isolated jumps, convergence near these jumps is marred by the *Gibbs phenomenon*: $S_p(f)$ always 'overshoots the mark' by about 9%, the area under the spurious peak tending to 0 as $p \to \infty$ but not its height [see Larmor (1934) for the history of this phenomenon].

By contrast, the *arithmetic mean* of the partial sums, also called the pth Cesàro sum,

$$C_p(f) = \frac{1}{p+1}[S_0(f) + \ldots + S_p(f)],$$

converges to f in the sense of the L^1 norm: $\|C_p(f) - f\|_1 \to 0$ as $p \to \infty$. If furthermore f is *continuous*, then the convergence is *uniform*, *i.e.* the error is bounded everywhere by a quantity which goes to 0 as $p \to \infty$. It may be shown that

$$C_p(f) = F_p * f,$$

where

$$F_p(x) = \sum_{|m| \leq p} \left(1 - \frac{|m|}{p+1}\right) \exp(2\pi i m x) = \frac{1}{p+1}\left[\frac{\sin(p+1)\pi x}{\sin \pi x}\right]^2$$

is the *Fejér kernel*. F_p has over D_p the advantage of being everywhere positive, so that the Cesàro sums $C_p(f)$ of a positive function f are always positive.

The de la Vallée Poussin kernel

$$V_p(x) = 2F_{2p+1}(x) - F_p(x)$$

has a trapezoidal distribution of coefficients and is such that $c_m(V_p) = 1$ if $|m| \leq p+1$; therefore $V_p * f$ is a trigonometric polynomial with the same Fourier coefficients as f over that range of values of m.

The Poisson kernel

$$\begin{aligned} P_r(x) &= 1 + 2\sum_{m=1}^{\infty} r^m \cos 2\pi m x \\ &= \frac{1 - r^2}{1 - 2r\cos 2\pi m x + r^2} \end{aligned}$$

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

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

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):

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

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 $p \to \infty$. The convolution is performed by multiplying the Fourier coefficients of f by those of α_p, so that one forms the quantities

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

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

$$\begin{aligned} \|f\|_1^2 &= \left(\int_0^1 |f(x)| \times 1 \,\mathrm{d}x\right)^2 \\ &\leq \left(\int_0^1 |f(x)|^2 \,\mathrm{d}x\right)\left(\int_0^1 1^2 \,\mathrm{d}x\right) = \|f\|_2^2 \leq \infty. \end{aligned}$$

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

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

and because the family of functions $\{\exp(2\pi i m x)\}_{m\in\mathbb{Z}}$ 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 $\{\exp(2\pi i m x)\}_{m\in\mathbb{Z}}$, the partial sum $S_p(f)$ is the best mean-square fit to f in the linear subspace of L^2 spanned by $\{\exp(2\pi i m x)\}_{|m|\leq p}$, 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 $|m| \to \infty$, say $|w_m| \leq C|m|^K$. Then the sequence $\{w_m/(2\pi i m)^{K+2}\}_{m\in\mathbb{Z}}$ is in ℓ^2 and even defines a *continuous* function $f \in L^2(\mathbb{R}/\mathbb{Z})$ and an associated tempered distribution $T_f \in \mathscr{D}'(\mathbb{R}/\mathbb{Z})$. 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 $|m| \to \infty$.

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 $\varphi \in \mathscr{E}(\mathbb{R}^n)$ be such that $\Phi = \mathscr{F}[\varphi]$ 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

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

references