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,

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

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,

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

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

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

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

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

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.

references