International Tables for Crystallography (2006). Vol. B, Section 1.3.2.6.9.3, pp. 43–44.

$$\sum_{\mathbf{x}\in\Lambda}\varphi(\mathbf{x}) = |\det \mathbf{A}|^{-1} \sum_{\boldsymbol{\xi}\in\Lambda^*} \mathscr{F}[\varphi](\boldsymbol{\xi}).$$

This identity, which also holds for $\bar{\mathscr{F}}$, is called the *Poisson summation formula*. Its usefulness follows from the fact that the speed of decrease at infinity of φ and $\mathscr{F}[\varphi]$ are inversely related (Section 1.3.2.4.4.3), so that if one of the series (say, the left-hand side) is slowly convergent, the other (say, the right-hand side) will be rapidly convergent. This procedure has been used by Ewald (1921) [see also Bertaut (1952), Born & Huang (1954)] to evaluate lattice sums (Madelung constants) involved in the calculation of the internal electrostatic energy of crystals (see Chapter 3.4 in this volume on convergence acceleration techniques for crystallographic lattice sums).

When φ is a multivariate Gaussian

$$\varphi(\mathbf{x}) = G_{\mathbf{B}}(\mathbf{x}) = \exp(-\tfrac{1}{2}\mathbf{x}^T\mathbf{B}\mathbf{x}),$$

then

$$\mathscr{F}[\varphi](\boldsymbol{\xi}) = |\det (2\pi\mathbf{B}^{-1})|^{1/2} G_{\mathbf{B}^{-1}}(\boldsymbol{\xi}),$$

and Poisson's summation formula for a lattice with period matrix $\mathbf{A}$ reads:

$$\sum_{\mathbf{m}\in\mathbb{Z}^n} G_{\mathbf{B}}(\mathbf{A}\mathbf{m}) = |\det \mathbf{A}|^{-1} |\det (2\pi\mathbf{B}^{-1})|^{1/2} \times \sum_{\boldsymbol{\mu}\in\mathbb{Z}^n} G_{4\pi^2\mathbf{B}^{-1}}[(\mathbf{A}^{-1})^T\boldsymbol{\mu}]$$

or equivalently

$$\sum_{\mathbf{m}\in\mathbb{Z}^n} G_C(\mathbf{m}) = |\det (2\pi\mathbf{C}^{-1})|^{1/2} \sum_{\boldsymbol{\mu}\in\mathbb{Z}^n} G_{4\pi^2\mathbf{C}^{-1}}(\boldsymbol{\mu})$$

with $\mathbf{C} = \mathbf{A}^T\mathbf{B}\mathbf{A}$.

1.3.2.6.8. *Convolution of Fourier series*

Let $S = R * S^0$ and $T = R * T^0$ be two Λ-periodic distributions, the motifs S^0 and T^0 having compact support. The convolution $S * T$ does not exist, because S and T do not satisfy the support condition (Section 1.3.2.3.9.7). However, the three distributions R, S^0 and T^0 do satisfy the generalized support condition, so that their convolution is defined; then, by associativity and commutativity:

$$R * S^0 * T^0 = S * T^0 = S^0 * T.$$

By Fourier transformation and by the convolution theorem:

$$\begin{aligned} R^* \times \mathscr{F}[S^0 * T^0] &= (R^* \times \mathscr{F}[S^0]) \times \mathscr{F}[T^0] \\ &= \mathscr{F}[T^0] \times (R^* \times \mathscr{F}[S^0]). \end{aligned}$$

Let $\{U_{\boldsymbol{\xi}}\}_{\boldsymbol{\xi}\in\Lambda^*}$, $\{V_{\boldsymbol{\xi}}\}_{\boldsymbol{\xi}\in\Lambda^*}$ and $\{W_{\boldsymbol{\xi}}\}_{\boldsymbol{\xi}\in\Lambda^*}$ be the sets of Fourier coefficients associated to S, T and $S * T^0 (= S^0 * T)$, respectively. Identifying the coefficients of $\delta_{\boldsymbol{\xi}}$ for $\boldsymbol{\xi}\in\Lambda^*$ yields the forward version of the convolution theorem for Fourier series:

$$W_{\boldsymbol{\xi}} = |\det \mathbf{A}| U_{\boldsymbol{\xi}} V_{\boldsymbol{\xi}}.$$

The backward version of the theorem requires that T be infinitely differentiable. The distribution $S \times T$ is then well defined and its Fourier coefficients $\{Q_{\boldsymbol{\xi}}\}_{\boldsymbol{\xi}\in\Lambda^*}$ are given by

$$Q_{\boldsymbol{\xi}} = \sum_{\boldsymbol{\eta}\in\Lambda^*} U_{\boldsymbol{\eta}} V_{\boldsymbol{\xi}-\boldsymbol{\eta}}.$$

1.3.2.6.9. *Toeplitz forms, Szegö's theorem*

Toeplitz forms were first investigated by Toeplitz (1907, 1910, 1911*a*). They occur in connection with the 'trigonometric moment problem' (Shohat & Tamarkin, 1943; Akhiezer, 1965) and probability theory (Grenander, 1952) and play an important role in several direct approaches to the crystallographic phase problem [see Sections 1.3.4.2.1.10, 1.3.4.5.2.2(*e*)]. Many aspects of their theory and applications are presented in the book by Grenander & Szegö (1958).

1.3.2.6.9.1. *Toeplitz forms*

Let $f \in L^1(\mathbb{R}/\mathbb{Z})$ be real-valued, so that its Fourier coefficients satisfy the relations $c_{-m}(f) = \overline{c_m(f)}$. The Hermitian form in $n+1$ complex variables

$$T_n[f](\mathbf{u}) = \sum_{\mu=0}^{n} \sum_{\nu=0}^{n} \overline{u_\mu} c_{\mu-\nu} u_\nu$$

is called the nth *Toeplitz form* associated to f. It is a straightforward consequence of the convolution theorem and of Parseval's identity that $T_n[f]$ may be written:

$$T_n[f](\mathbf{u}) = \int_0^1 \left| \sum_{\nu=0}^{n} u_\nu \exp(2\pi i\nu x) \right|^2 f(x)\,\mathrm{d}x.$$

1.3.2.6.9.2. *The Toeplitz–Carathéodory–Herglotz theorem*

It was shown independently by Toeplitz (1911*b*), Carathéodory (1911) and Herglotz (1911) that a function $f \in L^1$ is almost everywhere non-negative *if and only if* the Toeplitz forms $T_n[f]$ associated to f are positive semidefinite for all values of n.

This is equivalent to the infinite system of determinantal inequalities

$$D_n = \det \begin{pmatrix} c_0 & c_{-1} & \cdot & \cdot & c_{-n} \\ c_1 & c_0 & c_{-1} & \cdot & \cdot \\ \cdot & c_1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & c_{-1} \\ c_n & \cdot & \cdot & c_1 & c_0 \end{pmatrix} \geq 0 \quad \text{for all } n.$$

The D_n are called *Toeplitz determinants*. Their application to the crystallographic phase problem is described in Section 1.3.4.2.1.10.

1.3.2.6.9.3. *Asymptotic distribution of eigenvalues of Toeplitz forms*

The eigenvalues of the Hermitian form $T_n[f]$ are defined as the $n+1$ real roots of the characteristic equation $\det\{T_n[f-\lambda]\} = 0$. They will be denoted by

$$\lambda_1^{(n)}, \lambda_2^{(n)}, \ldots, \lambda_{n+1}^{(n)}.$$

It is easily shown that if $m \leq f(x) \leq M$ for all x, then $m \leq \lambda_\nu^{(n)} \leq M$ for all n and all $\nu = 1, \ldots, n+1$. As $n \to \infty$ these bounds, and the distribution of the $\lambda^{(n)}$ within these bounds, can be made more precise by introducing two new notions.

(i) *Essential bounds*: define ess inf f as the largest m such that $f(x) \geq m$ except for values of x forming a set of measure 0; and define ess sup f similarly.

(ii) *Equal distribution*. For each n, consider two sets of $n+1$ real numbers:

$$a_1^{(n)}, a_2^{(n)}, \ldots, a_{n+1}^{(n)}, \quad \text{and} \quad b_1^{(n)}, b_2^{(n)}, \ldots, b_{n+1}^{(n)}.$$

Assume that for each ν and each n, $|a_\nu^{(n)}| < K$ and $|b_\nu^{(n)}| < K$ with K independent of ν and n. The sets $\{a_\nu^{(n)}\}$ and $\{b_\nu^{(n)}\}$ are said to be equally distributed in $[-K, +K]$ if, for any function F over $[-K, +K]$,

$$\lim_{n\to\infty} \frac{1}{n+1} \sum_{\nu=1}^{n+1} [F(a_\nu^{(n)}) - F(b_\nu^{(n)})] = 0.$$

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