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

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:

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

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 *n*th *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 $[-K, +K]$,

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

 references