International Tables for Crystallography (2006). Vol. B, Section 1.3.2.7.1, pp. 45–46.

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):

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

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

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

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

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

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 $\{\exp(2\pi imx)\}_{m\in\mathbb{Z}}$ 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 $|m| \to \infty$, 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 $T_f \in \mathscr{D}'(\mathbb{R}/\mathbb{Z})$. 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

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

which is essentially Φ periodized by period lattice $\Lambda = (\Lambda^*)^*$, with period matrix $\mathbf{A}$.

Let us assume that Λ is such that the translates of K by different period vectors of Λ are disjoint. Then we may recover Φ from $R * \Phi$ by masking the contents of a 'unit cell' $\mathscr{V}$ of Λ (*i.e.* a fundamental domain for the action of Λ in $\mathbb{R}^n$) whose boundary does not meet K. If $\chi_{\mathscr{V}}$ is the indicator function of $\mathscr{V}$, then

$$\Phi = \chi_{\mathscr{V}} \times (R * \Phi).$$

Transforming both sides by $\bar{\mathscr{F}}$ yields

$$\varphi = \bar{\mathscr{F}}\left[\chi_{\mathscr{V}} \times \frac{1}{|\det \mathbf{A}|}\mathscr{F}[R^* \times \varphi]\right],$$

i.e.

$$\varphi = \left(\frac{1}{V}\bar{\mathscr{F}}[\chi_{\mathscr{V}}]\right) * (R^* \times \varphi)$$

since $|\det \mathbf{A}|$ is the volume V of $\mathscr{V}$.

This interpolation formula is traditionally credited to Shannon (1949), although it was discovered much earlier by Whittaker (1915). It shows that φ may be recovered from its sample values on Λ^* (*i.e.* from $R^* \times \varphi$) provided Λ^* is sufficiently fine that no overlap (or 'aliasing') occurs in the periodization of Φ by the dual lattice Λ. The interpolation kernel is the transform of the normalized indicator function of a unit cell of Λ containing the support K of Φ.

If K is contained in a sphere of radius $1/\Delta$ and if Λ and Λ^* are rectangular, the length of each basis vector of Λ must be greater than $2/\Delta$, and thus the sampling interval must be smaller than $\Delta/2$. This requirement constitutes the Shannon sampling criterion.

1.3.2.7.2. *Duality between subdivision and decimation of period lattices*

1.3.2.7.2.1. *Geometric description of sublattices*

Let $\Lambda_{\mathbf{A}}$ be a period lattice in $\mathbb{R}^n$ with matrix $\mathbf{A}$, and let $\Lambda_{\mathbf{A}}^*$ be the lattice reciprocal to $\Lambda_{\mathbf{A}}$, with period matrix $(A^{-1})^T$. Let $\Lambda_{\mathbf{B}}, \mathbf{B}, \Lambda_{\mathbf{B}}^*$ be defined similarly, and let us suppose that $\Lambda_{\mathbf{A}}$ *is a sublattice of* $\Lambda_{\mathbf{B}}$, *i.e.* that $\Lambda_{\mathbf{B}} \supset \Lambda_{\mathbf{A}}$ as a set.

The relation between $\Lambda_{\mathbf{A}}$ and $\Lambda_{\mathbf{B}}$ may be described in two different fashions: (i) multiplicatively, and (ii) additively.

(i) We may write $\mathbf{A} = \mathbf{BN}$ for some non-singular matrix $\mathbf{N}$ with integer entries. $\mathbf{N}$ may be viewed as the period matrix of the coarser lattice $\Lambda_{\mathbf{A}}$ with respect to the period basis of the finer lattice $\Lambda_{\mathbf{B}}$. It will be more convenient to write $\mathbf{A} = \mathbf{DB}$, where $\mathbf{D} = \mathbf{BNB}^{-1}$ is a rational matrix (with integer determinant since $\det \mathbf{D} = \det \mathbf{N}$) in terms of which the two lattices are related by

$$\Lambda_{\mathbf{A}} = \mathbf{D}\Lambda_{\mathbf{B}}.$$

(ii) Call two vectors in $\Lambda_{\mathbf{B}}$ *congruent modulo* $\Lambda_{\mathbf{A}}$ if their difference lies in $\Lambda_{\mathbf{A}}$. Denote the set of congruence classes (or 'cosets') by $\Lambda_{\mathbf{B}}/\Lambda_{\mathbf{A}}$, and the number of these classes by $[\Lambda_{\mathbf{B}} : \Lambda_{\mathbf{A}}]$. The 'coset decomposition'

$$\Lambda_{\mathbf{B}} = \bigcup_{\ell \in \Lambda_{\mathbf{B}}/\Lambda_{\mathbf{A}}} (\ell + \Lambda_{\mathbf{A}})$$

represents $\Lambda_{\mathbf{B}}$ as the disjoint union of $[\Lambda_{\mathbf{B}} : \Lambda_{\mathbf{A}}]$ translates of $\Lambda_{\mathbf{A}}$. $\Lambda_{\mathbf{B}}/\Lambda_{\mathbf{A}}$ is a finite lattice with $[\Lambda_{\mathbf{B}} : \Lambda_{\mathbf{A}}]$ elements, called the *residual lattice* of $\Lambda_{\mathbf{B}}$ modulo $\Lambda_{\mathbf{A}}$.

The two descriptions are connected by the relation $[\Lambda_{\mathbf{B}} : \Lambda_{\mathbf{A}}] = \det \mathbf{D} = \det \mathbf{N}$, which follows from a volume calculation. We may also combine (i) and (ii) into

$$\text{(iii)} \qquad \Lambda_{\mathbf{B}} = \bigcup_{\ell \in \Lambda_{\mathbf{B}}/\Lambda_{\mathbf{A}}} (\ell + \mathbf{D}\Lambda_{\mathbf{B}})$$

which may be viewed as the n-dimensional equivalent of the Euclidean algorithm for integer division: ℓ is the 'remainder' of the division by $\Lambda_{\mathbf{A}}$ of a vector in $\Lambda_{\mathbf{B}}$, the quotient being the matrix $\mathbf{D}$.

1.3.2.7.2.2. *Sublattice relations for reciprocal lattices*

Let us now consider the two *reciprocal lattices* $\Lambda_{\mathbf{A}}^*$ and $\Lambda_{\mathbf{B}}^*$. Their period matrices $(\mathbf{A}^{-1})^T$ and $(\mathbf{B}^{-1})^T$ are related by: $(\mathbf{B}^{-1})^T = (\mathbf{A}^{-1})^T\mathbf{N}^T$, where $\mathbf{N}^T$ is an integer matrix; or equivalently by $(\mathbf{B}^{-1})^T = \mathbf{D}^T(\mathbf{A}^{-1})^T$. This shows that the roles are reversed in that $\Lambda_{\mathbf{B}}^*$ *is a sublattice of* $\Lambda_{\mathbf{A}}^*$, which we may write:

$$\text{(i)}^* \qquad \Lambda_{\mathbf{B}}^* = \mathbf{D}^T\Lambda_{\mathbf{A}}^*$$

$$\text{(ii)}^* \qquad \Lambda_{\mathbf{A}}^* = \bigcup_{\ell^* \in \Lambda_{\mathbf{A}}^*/\Lambda_{\mathbf{B}}^*} (\ell^* + \Lambda_{\mathbf{B}}^*).$$

The residual lattice $\Lambda_{\mathbf{A}}^*/\Lambda_{\mathbf{B}}^*$ is finite, with $[\Lambda_{\mathbf{A}}^* : \Lambda_{\mathbf{B}}^*] = \det \mathbf{D} = \det \mathbf{N} = [\Lambda_{\mathbf{B}} : \Lambda_{\mathbf{A}}]$, and we may again combine (i)* and (ii)* into

$$\text{(iii)}^* \qquad \Lambda_{\mathbf{A}}^* = \bigcup_{\ell^* \in \Lambda_{\mathbf{A}}^*/\Lambda_{\mathbf{B}}^*} (\ell^* + \mathbf{D}^T\Lambda_{\mathbf{A}}^*).$$

1.3.2.7.2.3. *Relation between lattice distributions*

The above relations between lattices may be rewritten in terms of the corresponding *lattice distributions* as follows:

$$\text{(i)} \qquad R_{\mathbf{A}} = \frac{1}{|\det \mathbf{D}|}\mathbf{D}^\# R_{\mathbf{B}}^*$$

$$\text{(ii)} \qquad R_{\mathbf{B}} = T_{\mathbf{B}/\mathbf{A}} * R_{\mathbf{A}}$$

$$\text{(i)}^* \qquad R_{\mathbf{B}}^* = \frac{1}{|\det \mathbf{D}|}(\mathbf{D}^T)^\# R_{\mathbf{A}}^*$$

$$\text{(ii)}^* \qquad R_{\mathbf{A}}^* = T_{\mathbf{A}/\mathbf{B}}^* * R_{\mathbf{B}}^*$$

where

$$T_{\mathbf{B}/\mathbf{A}} = \sum_{\ell \in \Lambda_{\mathbf{B}}/\Lambda_{\mathbf{A}}} \delta_{(\ell)}$$

and

$$T_{\mathbf{A}/\mathbf{B}}^* = \sum_{\ell^* \in \Lambda_{\mathbf{A}}^*/\Lambda_{\mathbf{B}}^*} \delta_{(\ell^*)}$$

are (finite) residual-lattice distributions. We may incorporate the factor $1/|\det \mathbf{D}|$ in (i) and (i)* into these distributions and define

$$S_{\mathbf{B}/\mathbf{A}} = \frac{1}{|\det \mathbf{D}|}T_{\mathbf{B}/\mathbf{A}}, \quad S_{\mathbf{A}/\mathbf{B}}^* = \frac{1}{|\det \mathbf{D}|}T_{\mathbf{A}/\mathbf{B}}^*.$$

Since $|\det \mathbf{D}| = [\Lambda_{\mathbf{B}} : \Lambda_{\mathbf{A}}] = [\Lambda_{\mathbf{A}}^* : \Lambda_{\mathbf{B}}^*]$, convolution with $S_{\mathbf{B}/\mathbf{A}}$ and $S_{\mathbf{A}/\mathbf{B}}^*$ has the effect of *averaging* the translates of a distribution under the elements (or 'cosets') of the residual lattices $\Lambda_{\mathbf{B}}/\Lambda_{\mathbf{A}}$ and $\Lambda_{\mathbf{A}}^*/\Lambda_{\mathbf{B}}^*$, respectively. This process will be called 'coset averaging'. Eliminating $R_{\mathbf{A}}$ and $R_{\mathbf{B}}$ between (i) and (ii), and $R_{\mathbf{A}}^*$ and $R_{\mathbf{B}}^*$ between (i)* and (ii)*, we may write:

$$\text{(i}'\text{)} \qquad R_{\mathbf{A}} = \mathbf{D}^\#(S_{\mathbf{B}/\mathbf{A}} * R_{\mathbf{A}})$$

$$\text{(ii}'\text{)} \qquad R_{\mathbf{B}} = S_{\mathbf{B}/\mathbf{A}} * (\mathbf{D}^\# R_{\mathbf{B}})$$

$$\text{(i}'\text{)}^* \qquad R_{\mathbf{B}}^* = (\mathbf{D}^T)^\#(S_{\mathbf{A}/\mathbf{B}}^* * R_{\mathbf{B}}^*)$$

$$\text{(ii}'\text{)}^* \qquad R_{\mathbf{A}}^* = S_{\mathbf{A}/\mathbf{B}}^* * [(\mathbf{D}^T)^\# R_{\mathbf{A}}^*].$$

These identities show that *period subdivision* by convolution with

references