$$D_{\mathsf{H}}[\wp] = \det\{[F(\mathbf{h}_j - \mathbf{h}_k)]\}.$$

The Toeplitz–Carathéodory–Herglotz theorem given in Section 1.3.2.6.9.2 states that the converse is true: if $D_{\mathsf{H}}[\rho] \geq 0$ for all H, then $\wp$ is almost everywhere non-negative. This result is known in the crystallographic literature through the papers of Karle & Hauptman (1950), MacGillavry (1950), and Goedkoop (1950), following previous work by Harker & Kasper (1948) and Gillis (1948*a*,*b*).

Szegö's study of the asymptotic distribution of the eigenvalues of Toeplitz forms as their order tends to infinity remains valid. Some precautions are needed, however, to define the notion of a sequence (H_k) of finite subsets of indices tending to infinity: it suffices that the H_k should consist essentially of the reciprocal-lattice points $\mathbf{h}$ contained within a domain of the form $k\Omega$ (k-fold dilation of Ω) where Ω is a convex domain in $\mathbb{R}^3$ containing the origin (Widom, 1960). Under these circumstances, the eigenvalues $\lambda_\nu^{(n)}$ of the Toeplitz forms $T_{\mathsf{H}_k}[\wp]$ become equidistributed with the sample values $\wp_{\nu'}^{(n)}$ of $\wp$ on a grid satisfying the Shannon sampling criterion for the data in H_k (*cf.* Section 1.3.2.6.9.3).

A particular consequence of this equidistribution is that the geometric means of the $\lambda_\nu^{(n)}$ and of the $\wp_{\nu'}^{(n)}$ are equal, and hence as in Section 1.3.2.6.9.4

$$\lim_{k\to\infty}\{D_{\mathsf{H}_k}[\wp]\}^{1/|\mathsf{H}_k|} = \exp\left\{\int_{\mathbb{R}^3/\mathbb{Z}^3} \log \wp(\mathbf{x})\,\mathrm{d}^3\mathbf{x}\right\},$$

where $|\mathsf{H}_k|$ denotes the number of reflections in H_k. Complementary terms giving a better comparison of the two sides were obtained by Widom (1960, 1975) and Linnik (1975).

This formula played an important role in the solution of the 2D Ising model by Onsager (1944) (see Montroll *et al.*, 1963). It is also encountered in phasing methods involving the 'Burg entropy' (Britten & Collins, 1982; Narayan & Nityananda, 1982; Bricogne, 1982, 1984, 1988).

1.3.4.2.2. Crystal symmetry

1.3.4.2.2.1. Crystallographic groups

The description of a crystal given so far has dealt only with its invariance under the action of the (discrete Abelian) group of translations by vectors of its period lattice Λ.

Let the crystal now be embedded in Euclidean 3-space, so that it may be acted upon by the group $M(3)$ of rigid (*i.e.* distance-preserving) motions of that space. The group $M(3)$ contains a normal subgroup $T(3)$ of translations, and the quotient group $M(3)/T(3)$ may be identified with the 3-dimensional orthogonal group $O(3)$. The period lattice Λ of a crystal is a discrete uniform subgroup of $T(3)$.

The possible invariance properties of a crystal under the action of $M(3)$ are captured by the following definition: a *crystallographic group* is a subgroup Γ of $M(3)$ if

(i) $\Gamma \cap T(3) = \Lambda$, a period lattice and a normal subgroup of Γ;

(ii) the factor group $G = \Gamma/\Lambda$ is finite.

The two properties are not independent: by a theorem of Bieberbach (1911), they follow from the assumption that Λ is a discrete subgroup of $M(3)$ which operates without accumulation point and with a compact fundamental domain (see Auslander, 1965). These two assumptions imply that G acts on Λ through an integral representation, and this observation leads to a complete enumeration of all distinct Γ's. The mathematical theory of these groups is still an active research topic (see, for instance, Farkas, 1981), and has applications to Riemannian geometry (Wolf, 1967).

This classification of crystallographic groups is described elsewhere in these *Tables* (Wondratschek, 2005), but it will be surveyed briefly in Section 1.3.4.2.2.3 for the purpose of establishing further terminology and notation, after recalling basic notions and results concerning groups and group actions in Section 1.3.4.2.2.2.

1.3.4.2.2.2. Groups and group actions

The books by Hall (1959) and Scott (1964) are recommended as reference works on group theory.

(*a*) *Left and right actions*

Let G be a group with identity element e, and let X be a set. An *action* of G on X is a mapping from $G \times X$ to X with the property that, if $g\,x$ denotes the image of (g, x), then

(i) $(g_1g_2)x = g_1(g_2x)$ for all $g_1, g_2 \in G$ and all $x \in X$,

(ii) $ex = x$ for all $x \in X$.

An element g of G thus induces a mapping T_g of X into itself defined by $T_g(x) = gx$, with the 'representation property':

(iii) $T_{g_1g_2} = T_{g_1}T_{g_2}$ for all $g_1, g_2 \in G$.

Since G is a group, every g has an inverse g^{-1}; hence every mapping T_g has an inverse $T_{g^{-1}}$, so that each T_g is a permutation of X.

Strictly speaking, what has just been defined is a *left* action. A *right* action of G on X is defined similarly as a mapping $(g, x) \longmapsto xg$ such that

(i′) $x(g_1g_2) = (xg_1)g_2$ for all $g_1, g_2 \in G$ and all $x \in X$,

(ii′) $xe = x$ for all $x \in X$.

The mapping T'_g defined by $T'_g(x) = xg$ then has the 'right-representation' property:

(iii′) $T'_{g_1g_2} = T'_{g_2}T'_{g_1}$ for all $g_1, g_2 \in G$.

The essential difference between left and right actions is of course not whether the elements of G are written on the left or right of those of X: it lies in the difference between (iii) and (iii′). In a left action the product g_1g_2 in G operates on $x \in X$ by g_2 operating first, then g_1 operating on the result; in a right action, g_1 operates first, then g_2. This distinction will be of importance in Sections 1.3.4.2.2.4 and 1.3.4.2.2.5. In the sequel, we will use left actions unless otherwise stated.

(*b*) *Orbits and isotropy subgroups*

Let x be a fixed element of X. Two fundamental entities are associated to x:

(1) the subset of G consisting of all g such that $gx = x$ is a subgroup of G, called the *isotropy subgroup* of x and denoted G_x;

(2) the subset of X consisting of all elements gx with g running through G is called the *orbit* of x under G and is denoted Gx.

Through these definitions, the action of G on X can be related to the internal structure of G, as follows. Let G/G_x denote the collection of distinct left cosets of G_x in G, *i.e.* of distinct subsets of G of the form gG_x. Let $|G|$, $|G_x|$, $|Gx|$ and $|G/G_x|$ denote the numbers of elements in the corresponding sets. The number $|G/G_x|$ of distinct cosets of G_x in G is also denoted $[G : G_x]$ and is called the *index* of G_x in G; by Lagrange's theorem

$$[G : G_x] = |G/G_x| = \frac{|G|}{|G_x|}.$$