

2.1. STATISTICAL PROPERTIES OF THE WEIGHTED RECIPROCAL LATTICE

$$\lambda_u = \beta + \frac{1}{8\beta} - \frac{124}{3(8\beta)^3} + \frac{120928}{15(8\lambda)^5} - \frac{401743168}{105(8\lambda)^7} + \dots, \quad (2.1.8.15)$$

where $\beta = (u - \frac{1}{4})\pi$. For $u > 5$ the values given by equation (2.1.8.15) have a relative error less than 10^{-11} so that no refinement of roots of higher orders is needed (Shmueli *et al.*, 1984). Numerical computations of single Fourier–Bessel series are of course faster than those of the double Fourier series, but both representations converge fairly rapidly.

2.1.8.3. Simple examples

Consider the Fourier coefficient of the p.d.f. of $|E|$ for the centrosymmetric space group $P\bar{1}$. The normalized structure factor is given by

$$E = 2 \sum_{j=1}^{N/2} n_j \cos \vartheta_j, \quad \text{with } \vartheta_j = 2\pi \mathbf{h}^T \cdot \mathbf{r}_j, \quad (2.1.8.16)$$

and the Fourier coefficient is

$$C_k = \langle \exp(\pi i k \alpha E) \rangle \quad (2.1.8.17)$$

$$= \left\langle \exp \left[2\pi i k \alpha \sum_{j=1}^{N/2} n_j \cos \vartheta_j \right] \right\rangle \quad (2.1.8.18)$$

$$= \left\langle \prod_{j=1}^{N/2} \exp(2\pi i k \alpha n_j \cos \vartheta_j) \right\rangle \quad (2.1.8.19)$$

$$= \prod_{j=1}^{N/2} \langle \exp(2\pi i k \alpha n_j \cos \vartheta_j) \rangle \quad (2.1.8.20)$$

$$= \prod_{j=1}^{N/2} \left\{ (1/2\pi) \int_{-\pi}^{\pi} \exp(2\pi i k \alpha n_j \cos \vartheta) d\vartheta \right\} \quad (2.1.8.21)$$

$$= \prod_{j=1}^{N/2} J_0(2\pi k \alpha n_j). \quad (2.1.8.22)$$

Equation (2.1.8.20) is obtained from equation (2.1.8.19) if we make use of the assumption of independence, the assumption of uniformity allows us to rewrite equation (2.1.8.20) as (2.1.8.21), and the expression in the braces in the latter equation is just a definition of the Bessel function $J_0(2\pi k \alpha n_j)$ (*e.g.* Abramowitz & Stegun, 1972).

Let us now consider the Fourier coefficient of the p.d.f. of $|E|$ for the noncentrosymmetric space group $P1$. We have

$$A = \sum_{j=1}^N n_j \cos \vartheta_j \quad \text{and} \quad B = \sum_{j=1}^N n_j \sin \vartheta_j. \quad (2.1.8.23)$$

These expressions for A and B are substituted in equation (2.1.8.10), resulting in

$$C_{mn} = \left\langle \prod_{j=1}^N \exp[\pi i \alpha n_j (m \cos \vartheta_j + n \sin \vartheta_j)] \right\rangle \quad (2.1.8.24)$$

$$= \left\langle \prod_{j=1}^N \exp[\pi i \alpha n_j \sqrt{m^2 + n^2} \sin(\vartheta_j + \Delta)] \right\rangle \quad (2.1.8.25)$$

$$= \prod_{j=1}^N J_0(\pi \alpha n_j \sqrt{m^2 + n^2}). \quad (2.1.8.26)$$

Equation (2.1.8.24) leads to (2.1.8.25) by introducing polar coordinates analogous to those leading to equation (2.1.8.8), and equation (2.1.8.26) is then obtained by making use of the assumptions of independence and uniformity in an analogous manner to that detailed in equations (2.1.8.12)–(2.1.8.22) above.

The right-hand side of equation (2.1.8.26) is to be used as a Fourier coefficient of the double Fourier series given by (2.1.8.9). Since, however, this coefficient depends on $(m^2 + n^2)^{1/2}$ alone rather than on m and n separately, the p.d.f. of $|E|$ for $P1$ can also be represented by a Fourier–Bessel series [*cf.* equation (2.1.8.11)] with coefficient

$$D_u = \frac{1}{J_1^2(\lambda_u)} \prod_{j=1}^N J_0(\alpha n_j \lambda_u), \quad (2.1.8.27)$$

where λ_u is the u th root of the equation $J_0(x) = 0$.

2.1.8.4. A more complicated example

We now illustrate the methodology of deriving characteristic functions for space groups of higher symmetries, following the method of Rabinovich *et al.* (1991*a,b*). The derivation is performed for the space group $P\bar{6}$ [No. 174]. According to Table A1.4.3.6, the real and imaginary parts of the normalized structure factor are given by

$$A = 2 \sum_{j=1}^{N/6} n_j [C(hki)c(lz)]_j \\ = 2 \sum_{j=1}^{N/6} n_j \cos \tau_j \sum_{k=1}^3 \cos \alpha_{jk} \quad (2.1.8.28)$$

and

$$B = 2 \sum_{j=1}^{N/6} n_j [S(hki)c(lz)]_j \\ = 2 \sum_{j=1}^{N/6} n_j \cos \tau_j \sum_{k=1}^3 \sin \alpha_{jk}, \quad (2.1.8.29)$$

where

$$\begin{aligned} \alpha_{j1} &= 2\pi(hx_j + ky_j), \\ \alpha_{j2} &= 2\pi(kx_j + iy_j), \\ \alpha_{j3} &= 2\pi(ix_j + hy_j), \\ \tau_j &= 2\pi l z_j. \end{aligned}$$

Note that $\alpha_{j1} + \alpha_{j2} + \alpha_{j3} = 0$, *i.e.*, one of these contributions depends on the other two; this is a recurring problem in calculations pertaining to trigonal and hexagonal systems. For brevity, we write directly the general form of the characteristic function from which the functional form of the Fourier coefficient can be readily obtained. The characteristic function is given by