

On this basis, as Φ is varied from 0 to 90°, the general point L'_- traces out the line L'_-L_- in Fig. 2(c). At some value of Φ , this line will cross the plane through the $\Delta 2\theta$ axis. The λ locus is then OL_-^0 , in projection OL_-^0 . The whole of the $\Delta\lambda$ band interacts simultaneously and so the λ component makes a zero contribution to the 'counter' profile for this setting of Φ . The setting condition for Φ is that $\cos \Phi = -t$; see equation (4) in Mathieson (1985).

Hence, by the appropriate choice of Φ , one can bring any reflection with scattering angle θ_c to the ZWD condition. The only limitation is that $\theta_c \leq \theta_M$.

Discussion

While the classical 'parallel' condition has valuable properties for the measurement of reflectivity curves and for the establishment of accurate structure-factor values, there are restrictions in its use. Normally, one wishes to measure for a specimen crystal a number of different Bragg reflections which span a range of θ_c . If only one monochromator crystal is available, then measurement in the ZWD condition cannot be attempted. The alternative is to obtain a number of monochromator crystals with Bragg angles exactly matched to those of the specimen crystal - a task difficult in practice. The scheme outlined here would provide suitable flexibility to extend the capability of zero-wavelength-dispersion measurement.

Fig. 2, especially Fig. 2(c), shows that the range of application of the procedure lies within the region

$0 \leq \theta_c \leq \theta_M$. Hence the larger θ_M is, the wider is its range of application and the greater its usefulness. The advantage of high θ_M for matters of resolution has been advocated on many occasions - the present proposal would appear to provide further reason for the use of high- θ_M monochromator crystals.

To effect this type of measurement requires that the four-circle diffractometer necessary to orient the specimen crystal (and detector) be itself mounted in a cradle which is capable of rotation about the beam for the monochromator crystal at least over the range $\Phi = 0$ to 90°. Thus, the basic requirement is a five-circle device.

The procedure suggested here would appear to be of interest to some users of synchrotrons where ZWD operations could be of value to explore variability in reflectivity curves and hence extinction conditions; see Fig. 4 in Höche, Schulz, Weber, Belzner, Wolf & Wulf (1986).

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Functional Form of Some Ideal Hypersymmetric Distributions of Structure Factors

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Abstract

The hypercentric or hyperparallel distribution of structure factors of order n [Rogers & Wilson (1953). *Acta Cryst.* **6**, 439-449] can be expressed in terms of Meijer's G functions [Erdélyi (1953). (Editor.) *Higher Transcendental Functions*, Vol. I, Ch. V. New York: McGraw-Hill]:

$$P_n(F) = (2^{n-2} \pi^n \Sigma)^{-1/2} \\ \times G_{n-1,n}^{n,0}(F^2/2^n \Sigma | \frac{1}{2}, \dots, \frac{1}{2}; 0, 0, \dots, 0),$$

where F is the modulus of the structure factor. This reduces to the known centric and bicentric distributions for $n = 1, 2$.

Introduction

The simplest hypersymmetric distribution, the bicentric, was introduced by Lipson & Woolfson (1952). They expressed it as an integral and evaluated it numerically. Their work was extended to higher hypersymmetries (hypercentric and hyperparallel) by Rogers & Wilson (Wilson, 1952; Rogers & Wilson, 1953), who showed that the bicentric distribution could be expressed in terms of the known Bessel function K_0 . For the higher members of the series Rogers & Wilson gave integral representations, moments and Gram-Charlier expansions. The purpose of this note is to express the higher members in terms of the known but not very familiar G functions

(Meijer, 1941, 1946). A brief summary of their properties is given by Erdélyi (1953, Ch. V). They have had many applications in statistics, particularly in tests of significance (Mathai & Saxena, 1973, Ch. 6). With the introduction of 'exact' Fourier and Fourier-Bessel expressions (Shmueli, Weiss, Kiefer & Wilson, 1984; Weiss, Shmueli, Kiefer & Wilson, 1985; Shmueli, Weiss & Kiefer, 1985) the results are less interesting than they would have been if they had been obtained in 1953, but it seems worthwhile to place them on record. Like the acentric and centric distributions, they depend ultimately on the central-limit theorem (Wilson, 1949).

Derivation of the distribution function

Equation (12) of Rogers & Wilson (1953) is

$$P_n(F) = (2^n / \pi^{2n-1} \Sigma)^{1/2} \times \int_0^{\pi/2} \cdots \int_0^{\pi/2} \exp(-F^2 \sec^2 \varphi_2 \dots \sec^2 \varphi_n / 2^n \Sigma) \times \sec \varphi_2 \dots \sec \varphi_n d\varphi_2 \dots d\varphi_n, \quad n \geq 2, \quad (1)$$

where F is the modulus of the structure factor. With the substitutions

$$x_j = \sec^2 \varphi_j \quad (2)$$

this becomes

$$P_n(F) = (2^{n-2} \pi^{2n-1} \Sigma)^{-1/2} \times \int_1^\infty \cdots \int_1^\infty \exp(-F^2 x_2 \dots x_n / 2^n \Sigma) \times [x_2(x_2-1)]^{-1/2} dx_2 \dots [x_n(x_n-1)]^{-1/2} dx_n. \quad (3)$$

Performing the integration with respect to x_2 gives

$$P_n(F) = (2^{n-2} \pi^{2n-1} \Sigma)^{-1/2} \times \int_1^\infty \cdots \int_1^\infty \exp(-F^2 x_3 \dots x_n / 2^{n+1} \Sigma) \times K_0(F^2 x_3 \dots x_n / 2^{n+1} \Sigma) \times [x_3(x_3-1)]^{-1/2} dx_3 \dots [x_n(x_n-1)]^{-1/2} dx_n \quad (4)$$

[Gradshteyn & Ryzhik (1980), formula 3.383 (3)]. For $n=2$ the process stops here, there being no integrations left, and

$$P_2(F) = (\pi^3 \Sigma)^{-1/2} \exp(-F^2/8\Sigma) K_0(F^2/8\Sigma), \quad (5)$$

in agreement with equation (15) of Rogers & Wilson (1953). For $n=3$ the integration can be performed after replacing K_0 in (4) by its G -function equivalent

[Gradshteyn & Ryzhik (1980), formula 9.34 (6)]:

$$P_3(F) = (2\pi^4 \Sigma)^{-1/2} \int_1^\infty G_{1,2}^{2,0}(F^2 x_3 / 8\Sigma | \frac{1}{2}; 0, 0) \times [x_3(x_3-1)]^{-1/2} dx_3. \quad (6)$$

The integral is known [Gradshteyn & Ryzhik, formula 7.811 (3)], giving

$$P_3(F) = (2\pi^3 \Sigma)^{-1/2} G_{2,3}^{3,0}(F^2/8\Sigma | \frac{1}{2}, \frac{1}{2}; 0, 0, 0). \quad (7)$$

For $n > 3$ the process can be continued by the use of the same formula, each step increasing three of the affixes of G by unity and decreasing the power of π within the parentheses by unity, so that eventually

$$P_n(F) = (2^{n-2} \pi^n \Sigma)^{-1/2} \times G_{n-1,n}^{n,0}(F^2/2^n \Sigma | \frac{1}{2}, \dots, \frac{1}{2}; 0, 0, \dots, 0). \quad (8)$$

This reduces to the known centric and bicentric distributions for $n=1, 2$.

Computation of G functions

The computation of G functions has been treated by Mathai & Saxena (1973, Ch. 5). They obtain expansions in series of powers of $\log_e x$ with very complicated coefficients; these simplify somewhat in the present problem because there is only one independent affix n and the parameters are all either 0 or $\frac{1}{2}$. The asymptotic expansions are somewhat simpler, the leading term being

$$P_n(F) \approx (2^{n-2} \pi^n \Sigma)^{-1/2} (F^2/2^n \Sigma)^{-(n-1)/2} \times \exp(-F^2/2^n \Sigma). \quad (9)$$

For $n=1$ (the ideal centric distribution) this reduces to the correct form

$$P_1(F) = (2/\pi \Sigma)^{1/2} \exp(-F^2/2\Sigma) \quad (10)$$

and for $n=0$ (the ideal acentric distribution) it reduces to

$$P_0(F) = (2F/\Sigma) \exp(-F^2/\Sigma). \quad (11)$$

The correct form in (11) is perhaps unexpected, since the G function is not defined for negative affixes, and p takes the value -1 for $n=0$.

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Maximum Entropy Calculation of Electron Density with Native and Single Isomorphous Replacement Data

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Abstract

Maximum entropy is applied to the calculation of electron density maps from native and single isomorphous replacement (SIR) intensity data. Native intensity data alone at around 3 Å resolution are shown to be an insufficient constraint to give an interpretable map. When the method is applied to SIR data at the same resolution, either by direct selection between the 'most probable' phases, or by using both intensity data sets directly as constraints, the result is a significant improvement over a conventional 'best' map, as demonstrated by a calculation on data synthesized from a protein fragment. The robustness of the method is demonstrated by a series of calculations using increasingly noisy data.

1. Introduction

Recently, there has been increasing interest in applying maximum entropy in crystallography, ranging from the fundamental theory (Wilkins, Varghese & Lehmann, 1983; Livesey & Skilling, 1985) and the connection with direct methods (Bricogne, 1984) to the presentation of computational results. The latter have shown (*e.g.* Collins, 1982; Bricogne, 1984; Wei, 1985; Wilkins & Stuart, 1986; Navaza, 1986) that if structure factors are supplied to, say, 3 or 4 Å, then structure factor extension is possible (*i.e.* meaningful Fourier coefficients may be generated at reciprocal-lattice points beyond the resolution of the data provided). These calculations are analogous to those of Gull & Daniell (1978), in which the data were Fourier coefficients obtained by radio interferometer observations. However, our opinion is that if reliable multiple isomorphous replacement (MIR) phases are already

available to, say, 3 Å resolution, an electron density map produced by direct Fourier synthesis is usually interpretable. Whilst the map quality may be improved by structure factor extension beyond this figure, it is not essential for detailed model building. Delay in many protein structure determinations is frequently due to the difficulty of finding at least two derivatives which are sufficiently isomorphous to the native at 3 Å resolution. Several derivatives might be found which give good data to around 6 Å resolution, but not beyond, either because the crystals diffract poorly, or because the structure is disturbed locally by the inclusion of the heavy atoms so that it becomes non-isomorphous at higher resolution. Many techniques have evolved to make use of partly phased data, such as the use of non-crystallographic symmetry averaging, which has had great success in icosahedral virus structure determination (Harrison, Olson, Schutt, Winkler & Bricogne, 1978; Hogle, Chow & Filman, 1985; Rossmann *et al.*, 1985), where there are a large number of subunit copies in the asymmetric unit. However, such methods cannot be used in the more general problem without symmetry. Another approach has been to combine isomorphous replacement and direct methods (Hauptman, 1982), which, like many established direct methods, requires the assumption of atomicity, and will almost certainly lose power at lower resolution.

In previous work (Bryan, Bansal, Folkhard, Nave & Marvin, 1983), maximum entropy was applied to the calculation of the electron density of the coat protein of the filamentous virus Pfl from fibre diffraction data. Data from the native structure to 4 Å resolution and a single isomorphous derivative to 5 Å resolution were available (Nave *et al.*, 1981). The finite radius of a filamentous structure implies continuity of the structure factors as a function of layer-line radius, which is not ensured if the conventional

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