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The Correction of Resolution Errors in Small Angle Scattering Using Hermite Functions

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In a generalization of Guinier's approximation, the scattering functions in small angle scattering are represented by series of Hermite orthonormal functions. This allows a general solution of the slit height problem in terms of a simple coefficient formalism. To correct the slit width resolution error and the polychromatic effect on the basis of Hermite functions, orthonormal systems are constructed which lead to recurrence relations for the coefficients appearing in the solution. The methods have been numerically tested for various types of functions.

Introduction

The principal object of small angle scattering experiments is to get evidence of spatial correlations between the scattering centres of the physical system. Indirectly, such evidence may be found by comparison of the experimental distributions of scattered intensity with model distributions calculated from hypothetical configurations. This procedure requires a certain *a priori* knowledge of the spatial structure of the physical system.

The most general form of evidence from elastic small angle scattering is contained in the correlation function $g(\mathbf{r})$ represented by the Fourier transform of the scattering function, $S(\mathbf{x})$. If we restrict considerations to isotropic systems, the characteristic scattering function $S(\mathbf{x})$ depends only upon the absolute value of the scattering vector $\mathbf{x}=4\pi\lambda^{-1}\sin(\theta/2)$ (λ=wavelength, θ=scattering angle). If the correlation function is to be completely and exactly determined, the accurate shape of $S(\mathbf{x})$ in the whole range $0\le\mathbf{x}<\infty$ must be available. Unfortunately, measurements of intensity distributions only give limited information about $S(\mathbf{x})$ on a finite range of $\mathbf{x}$. In order to obtain sufficient scattered intensity the experimental conditions are usually far from the ideal case of a point-like primary spot produced by strictly monochromatic radiation. Wavelength distribution in the primary beam and finite angular divergence are the origins of resolution errors in the scattering distributions. Compared with the true shape of the scattering function $S(\mathbf{x})$ the experimental intensity distribution may be substantially distorted so that no direct evidence of $S(\mathbf{x})$ and of the correlations within the scattering system can be obtained. We describe the detector plane by a coordinate system (h,u), where h may be the reduced angular variable, $h=2p\cdot\sin(\theta/2)$ (p is a scaling parameter determined by the experimental design), and u is defined as perpendicular to h. We now postulate the wavelength distribution to be independent of the point (h,u) in the primary spot, and the intensity distribution in the horizontal direction along h to be independent of the distribution along u, and *vice versa*; thus the primary intensity is considered to be separable with regard to the wave number $\mathbf{k}$ and the variables h and u. If $i_B(h)$ and $i_H(u)$ are the so-called slit width and slit height weighting functions, and $z(\mathbf{k})$ is the primary 'momentum' distribution, where $\mathbf{k}=2\pi(p\lambda)^{-1}$, the relation:

$$i_0(h,u,\mathbf{k})=i_B(h)\cdot i_H(u)\cdot z(\mathbf{k})$$

may be assumed to hold. (The distributions may be taken to be normalized.) Then the scattered intensity distribution in the detector plane will be proportional to the following expression:

$$V(h)=\iiint i_B(h')i_H(u)z(\mathbf{k})\cdot S(\mathbf{k}\cdot\sqrt{(h-h')^2+u^2})\times d\mathbf{k}dudh'\,. \quad (1)$$

Thus the resolution errors are mathematically represented by three distinct integral equations. The polychromatic effect is described by the equation:

$$\mathscr{F}(h)=\int_0^\infty z(\mathbf{k})\cdot S(\mathbf{k}\cdot h)d\mathbf{k}\,. \quad (2)$$

Assuming a slit arrangement that behaves according to (1), the originally two-dimensional convolution problem of the geometrical distortions can be separated into the slit width effect,

$$V(h)=\int i_B(h')\cdot G(h-h')dh'\,, \quad (3)$$

and the slit height effect:

$$G(h)=\int i_H(u)\cdot\mathscr{F}(\sqrt{h^2+u^2})du\,. \quad (4)$$

Small angle scattering means scattering into an angular region where the approximation $h=p\theta$ holds; say $\theta<10^{-1}$ radian. Thus the ranges of θ and $\mathbf{x}$ may formally be extended to $-\infty<\theta,\mathbf{x}<\infty$. The integration boundaries in (3) and (4) are then defined by $-\infty$ and $+\infty$.

In various ways, many authors have dealt with these resolution errors. A survey of the literature can be found in the thesis of Hossfeld (1967). Contrary to the X-ray scattering situation, the smearing effect due to polychromatic radiation can be very important in neutron small angle scattering (Armbruster, Maier, Scherm, Schmatz & Springer, 1966). Luzzati (1957) showed that by substituting $h=\exp(t)$ and $\mathbf{k}=\exp(\mathbf{v})$, equation (2) is transformed into a convolution type equation equivalent to (3). This type of equation can be solved in principle by a Fourier transformation. However, we have not been able to find an explicit example of wavelength correction in the literature.

Provided that a slit arrangement is used, the slit width effect is often negligible compared with the alteration of scattering functions as a result of the slit height. Expansion of (3) by Fourier transforms always greatly magnifies the errors in the data, so this is not ordinarily a practical method. For slit width correction Taylor & Schmidt (1967) recently used the method of Sauder (1966), applying a Taylor series expansion, but this method needs at least double differentiation of the experimental data. Lake (1967) developed an iterative computer method starting with a trial function for simultaneous correction of slit-width and slit-height effects with arbitrary weighting functions.

Closed analytic solutions of the slit height equation were found by Guinier & Fournet (1947) and DuMond (1947) for infinite slit height, and by Kratky, Porod & Kahovec (1951) for the Gaussian type of slit height function. On these solutions almost all numerical methods have been based. Mazur & Wims (1966) recently derived a formal solution for arbitrary slit height functions. However, this method seems to be too unwieldy to be very useful in practice, and it has not, as yet, been numerically tested. So, excepting Lake's simultaneous iteration method, the convergence of which strongly depends upon the strength of the distortion effects, there is no practical method generally applicable to error correction in small angle scattering.

Representation by Hermite functions

The objective of any unsmearing operation is the appropriate transformation of a measured distribution into a scattering function $S(\mathbf{x})$. The result always has some degree of uncertainty, which depends upon the transformation of the statistical errors of the measured function and also upon our knowledge of the resolution functions.

An adequate method for handling distortion problems should satisfy the following requirements: (1) For the discrete set of experimental data [we neglect continuous recording methods which imply additional distortions (Hossfeld, 1966)] an appropriate representation should be found which accords with the actual functional character of scattering distributions. The information given by discrete sampling points should transform to a reduced number of variables now representing some functional distribution. A representation must take into account the possible functional types in small angle scattering, and should be simply Fourier transformed. (2) The detail of such a representation must be consistent with the statistics of the data, bearing in mind the use of least-squares fitting methods. (3) Distortion corrections based upon such a representation must be subject to a discussion of error propagation. (4) Correction methods should be suitable for computers.

These requirements are met by series expansions of the complete orthonormal system of Hermite functions:

$$\psi_{2n+s}^{(X)}=\left(\sum_{v=0}^{n} b_{2v+s}^{(2n+s)}X^{2v+s}\right).\exp(-X^2/2)\,, \qquad (5)$$

$n=0,1,2,\ldots;\ s=0$ or 1, where the $b_m^{(l)}$ are characteristic coefficients (Szegö, 1959). Hermite functions are invariant against Fourier transformation (Titchmarsh, 1948). Thus the correlation function $g(\mathbf{r})$ is easily expressed in terms of the expansion coefficients of the scattering function $S(\mathbf{x})$ (Hossfeld, 1967). Since the zero order Hermite function is a Gaussian, the Hermite expansion is equivalent to an expansion for perturbations of Guinier's approximation. Because of its completeness, the representation of scattering distributions by finite sums of Hermite functions can be made consistent with statistics according to the method of least squares. All experimental information is transformed into discrete expansion coefficients and correction methods on this basis will reduce to simple coefficient algebra.

Theory

In the following we give a closed treatment of the resolution errors by means of Hermite functions. At first we consider the slit height effect described by (4). We want to find the solution function $\mathscr{F}(h)$ as a series expansion of Hermite functions. Therefore $G(h)$ may be expanded to an index N according to the experimental accuracy of the data:

$$G(h)=\sum_{n=0}^{N} g_{2n}\psi_{2n}(h)\,,$$
$$g_{2n}=\int_{-\infty}^{\infty} G(h)\psi_{2n}(h)dh\,. \qquad (6)$$

Since all problems in isotropic small angle scattering are symmetrical, only Hermite functions of even order need to be considered. If we insert the postulated series expansion

$$\mathscr{F}(h)=\sum_{n=0}^{N} C_{2n}\psi_{2n}(h) \qquad (7)$$

into (4) we are able to separate the variables h and u. Using the explicit formula (5) for the Hermite functions we find after interchanging summation and integration:

$$G(h)=\sum_{K=0}^{N}\left(\sum_{n=K}^{N} C_{2n}\sum_{v=K}^{n} b_{2v}^{(2n)}A_{v,K}\right)h^{2K}.\exp(-h^2/2)\,, \quad (8)$$

where

$$A_{v,K}=\binom{v}{K}\int_{-\infty}^{\infty} i_H(u)\,.\,u^{2(v-K)}\exp(-u^2/2)du\,. \quad (9)$$

On the other hand we get from (6)

$$G(h)=\sum_{K=0}^{N}\left(\sum_{n=K}^{N} g_{2n}b_{2K}^{(2n)}\right)h^{2K}\,.\,\exp\left(-h^2/2\right)\,. \quad (10)$$

Comparison of equal powers of h in (8) and (10) yields a recurrence formula for the coefficients:

$$C_{2N}=\frac{g_{2N}}{A_{N,N}}\,;$$

$$C_{2K}=\frac{1}{b_{2K}^{(2K)}A_{K,K}}\left(\sum_{n=K}^{N} g_{2n}b_{2K}^{(2n)} - \sum_{n=K+1}^{N} C_{2n}\sum_{v=K}^{n} b_{2v}^{(2n)}A_{v,K}\right) \quad (11)$$

for $K=N-1,\ N-2,\ \ldots,\ 0$. Using (7), the slit height corrected scattering distribution $\mathscr{F}(h)$ may be calculated. The special shape of the slit height function $i_H(u)$ enters only into the triangular matrix $A_{v,K}$, a fact emphasizing the generality of this correction method. Of course, this way of solving type (4) equations can be extended to other problems, provided that the coupled functions satisfy certain integrability conditions concerning the expansion in Hermite polynomials.

A correction method for the slit width effect which finally arrives at a set of coefficients g_{2n} of an Hermite series expansion will be very useful in enabling an immediate slit height correction to be made according to (11). (The 'folding' theorem cannot reasonably be applied to this end.) If we postulate the solution $G(h)$ of (3) to be expanded in an Hermite series with appropriate convergence properties:

$$G(h)=\sum_{n=0}^{N} g_{2n}\psi_{2n}(h)\,, \quad (12)$$

we find after inserting (12) into (3)

$$V(h)=\sum_{n=0}^{N} g_{2n}\Phi_{2n}(h)\,, \quad (13)$$

where $\Phi_{2n}(h)$ are the Hermite functions $\psi_{2n}(h)$ folded with $i_B(h)$. These new functions are no longer orthogonal, but they remain linearly independent. Thus we can apply Schmidt's method (Morse & Feshbach, 1953) to orthonormalize the $\Phi_{2n}(h)$, constructing step-wise an orthonormal system $\varphi_{2n}(h)$, $n=0,1,\ldots$ The Φ_{2n} are related to the φ_{2n} by a triangular matrix T

$$\Phi_{2n}(h)=\sum_{m=0}^{n} T_{2n,2m}\,.\,\varphi_{2m}(h)\,, \quad (14)$$

where

$$T_{2n,2m}=\int_{-\infty}^{\infty}\Phi_{2n}(h)\,.\,\varphi_{2m}(h)dh\,,\ m\le n\,. \quad (15)$$

Then (13) yields

$$V(h)=\sum_{m=0}^{N}\left(\sum_{n=m}^{N} g_{2n}T_{2n,2m}\right).\,\varphi_{2m}(h)\,. \quad (16)$$

Now we expand the experimental curve $V(h)$ for the $\varphi_{2n}(h)$ according to its accuracy, thus determining the truncation index N:

$$V(h)=\sum_{n=0}^{N} v_{2n}\varphi_{2n}(h)\,;$$

$$v_{2n}=\int_{-\infty}^{\infty} V(h)\varphi_{2n}(h)dh\,; \quad (17)$$

comparison of expansion coefficients yields a recurrence formula for the g_{2n}:

$$g_{2N}=\frac{v_{2N}}{T_{2N,2N}}\,;$$

$$g_{2n}=\frac{1}{T_{2n,2n}}\left(v_{2n}-\sum_{m=n+1}^{N} g_{2m}T_{2m,2n}\right), \quad (18)$$

$n=N-1,\ N-2,\ \ldots,\ 0$. This method has the advantage of being adapted to the particular convolution problem by constructing a set of orthonormal functions which contain the special slit-width weighting distribution, provided that the postulated Hermite expansion of the solution is still reasonable. The set of g_{2n} can now be used to perform slit height correction if necessary.

In the same manner the equation for this effect due to polychromaticity can be solved. Inserting a postulated series expansion of the scattering function,

$$S(\mathbf{x})=\sum_{n=0}^{N} S_{2n}\psi_{2n}(\mathbf{x}) \quad (19)$$

into equation (2), and orthonormalizing the resulting Hermite functions distorted by $z(k)$, we again arrive at a recurrence relation for the solution coefficients:

$$S_{2N}=\frac{j_{2N}}{D_{2N,2N}}\,;$$

$$S_{2n}=\frac{1}{D_{2n,2n}}\left(j_{2n}-\sum_{m=n+1}^{N} S_{2m}D_{2m,2n}\right), \quad (20)$$

$n=N-1,\ N-2,\ \ldots,\ 0$. The triangular matrix D is analogous to T in (15). The j_{2n}'s are the coefficients of the experimental or collimation-corrected distribution $\mathscr{F}(h)$ expanded for orthonormal functions established by Schmidt's method. The truncation index N is determined by the statistics of $\mathscr{F}(h)$.

On expanding a Gaussian function $\exp\left(-a^2x^2/2\right)$ in terms of Hermite functions, all coefficients will vanish, with the exception of the zero order coefficient, if $a=1$. Thus the Hermite polynomial expansion of any Gaussian-like function will converge rapidly, after suitable transformation of the x-scale. Since in small angle scattering Guinier's approximation of scattering distributions has proved to be a useful representation we can improve the series convergence of Hermite expansions by taking a Gaussian shape as the first approximation. In order to adapt the scale of any distribution $f(x)$ we use the variance

$$\sigma_f^2=\frac{\int f(x)\,.\,x^2dx}{\int f(x)dx}$$

as a representative. Transforming $x^*=x/\sigma_f$, we find $\sigma^2_{f*}=1$ equivalent to the variance of the zero order Hermite function. In slit height correction, rapid convergence of the solution series $\mathscr{F}(h)$ is simply achieved by a rapidly convergent expansion of $G(h)$ after transforming the h-scale according to $\sigma^2_G\sim 1$. In order to optimize series convergence in slit width or wavelength distortion correction, we use moment relations of the respective integral equations. Transforming the h-scale by $h^*=h/(\sigma^2_V-\sigma^2_I)^{1/2}$, we adapt the variance of the slit width solution function $G(h)$ to that of $\psi_0(h)$, thus choosing an appropriate range of h for the Hermite representation (which is also adjusted for simultaneous slit-height correction if necessary). Using the moment relation of (2) for the variances of $\mathscr{F}(h)$ and $S(\mathbf{x})$, which is easily established, we adapt the $\mathbf{x}$-scale to $\psi_0(\mathbf{x})$ by transforming $h^*=h\,.\,\langle k^{-3}\rangle^{1/2}/(\langle k^{-1}\rangle\sigma^2_{\mathscr{F}})^{1/2}$ where

$$\langle k^{-m}\rangle=\int_0^\infty k^{-m}\,.\,z(k)dk\ .$$

By transformation of the h-scale the correction formalism is not changed. All scaling factors are calculated from experimental data.

Usually the statistical errors of scattered intensity measurements cannot be neglected. It is therefore important to consider carefully the propagation of errors during the process of resolution error correction. Since the Hermite function methods reduce to a simple recurrence formalism, error propagation can be discussed in a straightforward manner; the recurrence relations (11), (18) or (20) are used if the mean square errors of the g_{2n}, v_{2n} or j_{2n} respectively are known, while statistical errors in the weighting distributions are neglected (Hossfeld, 1967). Since expanding for orthonormal functions is equivalent to curve fitting by the method of least squares we are able to apply this well known formalism (Linnik, 1961) to calculate the mean square errors of g_{2n}, v_{2n} or j_{2n}.

However, using certain properties of orthonormal functions, and assuming statistical independence of the data, we can estimate the (co)variances of expansion coefficients in a direct way. Following Porteus (1962), and postulating that the sampling-point spacing of any experimental distribution, $f(x)$, to be expanded be much smaller than the distance between the narrowest zeros of the highest-index orthonormal function used, the (co)variances of the general expansion coefficients q_{2n} are given by

$$\langle \Delta q_{2n}\Delta q_{2m}\rangle=\int_{-\infty}^{\infty}\langle \Delta^2 f(x)\rangle\,.\,\chi_{2n}(x)\chi_{2m}(x)dx\ , \quad (22)$$

where $\chi_{2n}(x)$ are the orthonormal functions in question and $\langle \Delta^2 f(x)\rangle$ represents the estimated mean square error of $f(x)$. If $\langle \Delta^2 f(x)\rangle$ can be assumed to vary slowly with x compared with $\chi_{2n}\chi_{2m}$ the right hand side of (22) will vanish for $n\neq m$ because of orthogonality. Thus only the variances $\langle \Delta^2 q_{2n}\rangle$ need to be taken into account for error propagation.

Numerical results

For the purpose of numerical tests and application to experimental data, three Fortran programs have been established from the correction methods developed here on the basis of Hermite functions. In order to demonstrate the efficiency of the methods, various types of scattering functions were smeared out by typical weighting functions according to the integral equations (2), (3), and (4). The distorted curves were calculated where possible by analytical quadrature, but otherwise numerically. The correction methods of this paper were applied to these distributions, and the resulting shapes were compared with the exact scattering functions.

In Fig. 1(*a*)–(*c*) three examples are shown of slit height correction performed with rectangular slit height functions $i_H(u)$ of various heights. Fig. 1(*a*) exhibits a peak-shaped scattering function $\mathscr{F}(h)$ represented by a superposition of 6 Hermite functions ($n=0$ to 5) strongly distorted by the finite slit height. In the logarithmic scale over several orders of magnitude the agreement of the theoretical curve and the numerical values of the corrected function indicated by crosses becomes evident. In Fig. 1(*b*) the exact scattering function of a sphere (Beeman, Kaesberg, Anderegg & Webb, 1957) is compared with the numerical results obtained from corrections of two differently distorted functions $G(h)$. From these examples the influence of the sampling interval Δh of the input data on the quality of the slit height correction can be seen. Although the curve $G_2(h)$ had been smeared by a slit twice as high as for $G_1(h)$, the minima of the solution function are much better resolved because of a higher density of sampling points. The deviations on the right hand side of Fig. 1(*b*) are almost totally caused by the information loss due to the finite 'measuring range' used (Hossfeld & Maier, 1967). However, slit height correction by Hermite functions has yielded very good agreement with the theoretically expected curve within a range of at least six maxima and covering about six orders of magnitude. Fig. 1(*c*) shows the potentialities of the slit height correction method in the case of the slowly decreasing function $(\sin ah/ah)^2$. Because of its strong wings this function suffers appreciable information loss by the slit height effect. Nevertheless, performing the resolution correction by the Hermite function method yields good resolution of the minima and maxima up to the end of the h-range used, where information loss consequent on the finite range again becomes important.

For a first application of this correction method to experimental small angle scattering data it seemed reasonable to choose results taken with strictly monochromatic radiation and negligible slit width. Accordingly we used as $G(h)$ the X-ray small angle scattering of a latex, observed by Bonse & Hart (1965, 1966) with a high-resolution diffractometer. Two results of the slit height correction procedure with assumed rectangular weighting functions of various heights are shown in Fig. 2(*a*). The mean value of the diameter of the latex spheres, $D=0{\cdot}254\pm0{\cdot}014$ μm, obtained from the minima and maxima of the corrected curves exactly agrees with that value determined by Bonse & Hart after comparing the experimental data with artificially distorted scattering functions for spheres. $\mathscr{F}_2(h)$ seems to be slightly over-corrected, since its minima become appreciably negative with increasing h. Compared to the scattering function of spheres in Fig. 1(*b*) the data of Fig. 2(*a*) show that the latex sample exhibits an appreciable 'interparticle effect'. In Fig. 2(*b*) the theoretical self-correlation function of a sphere is compared with the correlation function $g(\mathbf{r})$ calculated by Fourier transformation of $\mathscr{F}_1(h)$. The peak related to next neighbours which arises in the region $\mathbf{r}/R=3$ is due to the interparticle effect.

In Fig. 3 two examples of slit width correction performed with a Fortran program of the Hermite function method are shown. In Fig. 3(*a*) a narrow Gaussian function substantially broadened by a Gaussian slit width function is subjected to numerical unfolding.

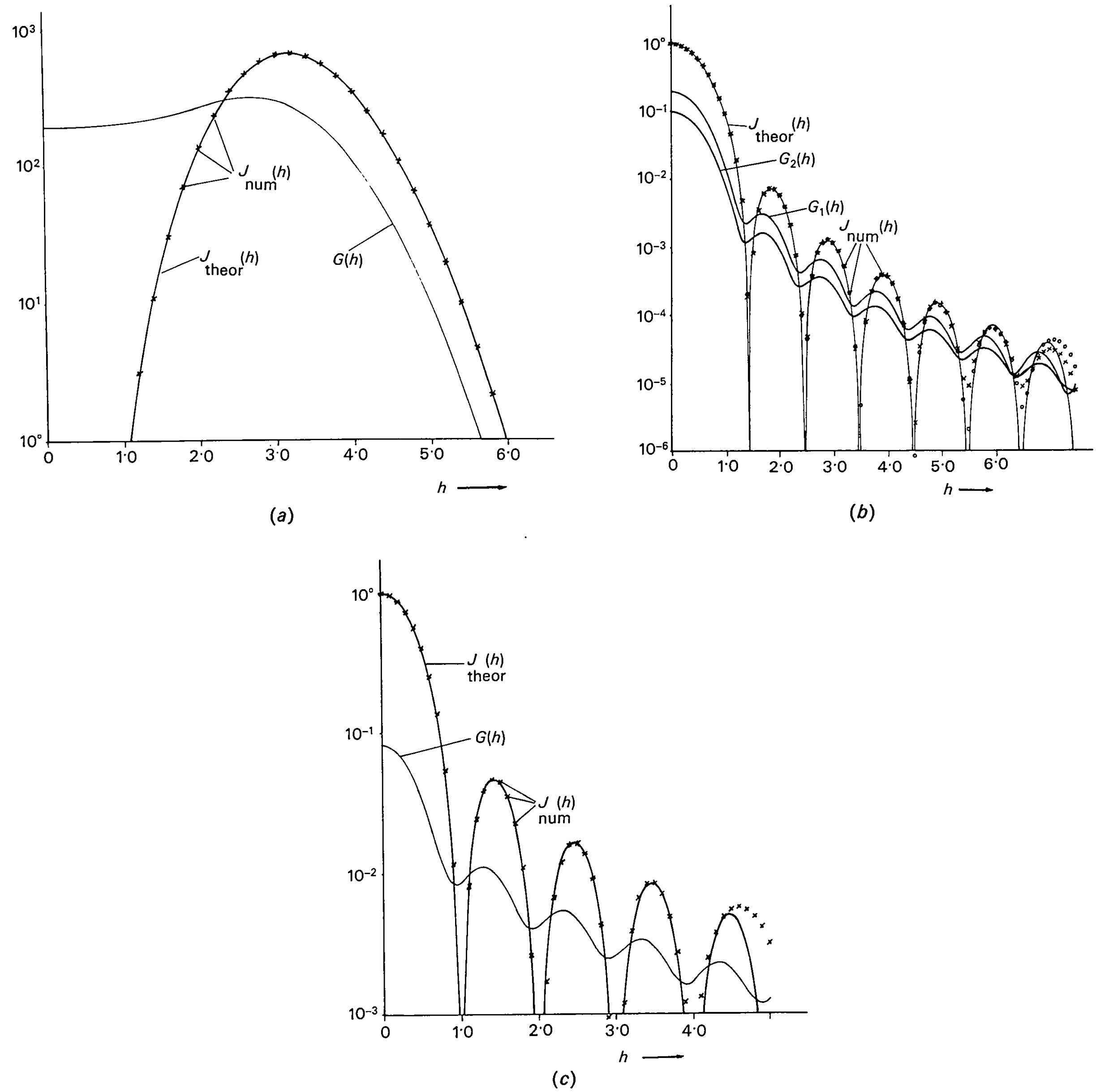

Fig. 1. Slit height correction by the Hermite function method: (*a*) $J_{\text{theor}}(h)=h^{10}\exp(-h^2/2)$, $i_H(u)=u^{-1}{}_M$, $|u|\le u_M$, $u_M=6$; (*b*) $J_{\text{theor}}(h)=9\,(\sin x-x\cdot\cos x)^2/x^6$, $x=\pi h$, $i_H(u)=u^{-1}{}_M$, $|u|\le u_M$; × × × $u_M=3$, $\Delta h=0{\cdot}15$; ○○○ $u_M=6$, $\Delta h=0{\cdot}10$; (*c*) $J_{\text{theor}}(h)=(\sin\pi h/\pi h)^2$, $i_H(u)=u^{-1}{}_M$, $|u|\le u_M$, $u_M=6$.

The numerical values of the corrected scattering function, indicated by crosses, agree very well with the theoretically expected curve to well below 10^{-4}. The results do not exhibit any influence of series truncation or finite h-range. In Fig. 3(*b*) the minimum of the undistorted curve $G_{\text{theor}}(h)$ is almost totally smeared out by the slit width effect resulting from a Gaussian weighting function; nevertheless the numerical results for the corrected function, indicated by crosses, are again satisfactory. Over the whole range the agreement with the theoretical function is better than can be seen with the logarithmic scale used.

For numerical experiments on the effect of polychromaticity, scattering functions of the type $S(x)=C(x/b)^{2n}\,.\,\exp(-x^2/b^2)$ were smeared out according to (3) by use of weighting functions $z(k)$ having a generalized Maxwellian shape $z(k)=Z_0\,.\,k^{m-2}\,.\,\exp(-\Lambda^2k^2)$. This process yielded wavelength-distorted curves of the form:

$$\mathscr{F}(h)=C_0\cdot\frac{\left(\frac{h}{\Lambda b}\right)^{2n}}{\left[1+\left(\frac{h}{\Lambda b}\right)^2\right]^{1/2(2n+m-1)}}\,. \tag{23}$$

We applied the Hermite function method for various n, m, b, and Λ. In order to avoid systematic errors during orthonormalization it is necessary to take a sufficiently large h-range. To diminish truncation effects it is preferable to interpolate linearly the experimental $z(k)$ and to perform piecewise analytical quadratures instead of numerical integrations for orthonormalizing. In Fig. 4(*a*), the small deviations on the wing of the solution $S(\mathbf{x})$ are truncation effects arising from the orthonormalization procedure, but the agreement with the theoretical shape is still very good in the significant region. Fig. 4(*b*) again demonstrates the strong distortion of the scattering function for increasing h. The numerical results agree with the sharp peak shape of the true curve, emphasizing the efficiency of the Hermite function method.

For wavelength corrections and slit width corrections the distorted distributions were represented by superpositions of 15 orthonormal functions, established by Schmidt's method. For slit height corrections 20 Hermite functions were used for the expansion of $G(h)$. The test runs shown in Figs. 1–4 were performed with the IBM 7090/1410 of the I.I.M. of the University of Bonn. Of course, the execution time strongly depends upon the number of orthonormal functions, ranging from a few seconds to some minutes for N about 20 using the IBM 7090.

Conclusions

The representation of scattering functions in small angle scattering by series of Hermite functions allows for a closed treatment of the geometric resolution errors caused by the finite height and width of collima-

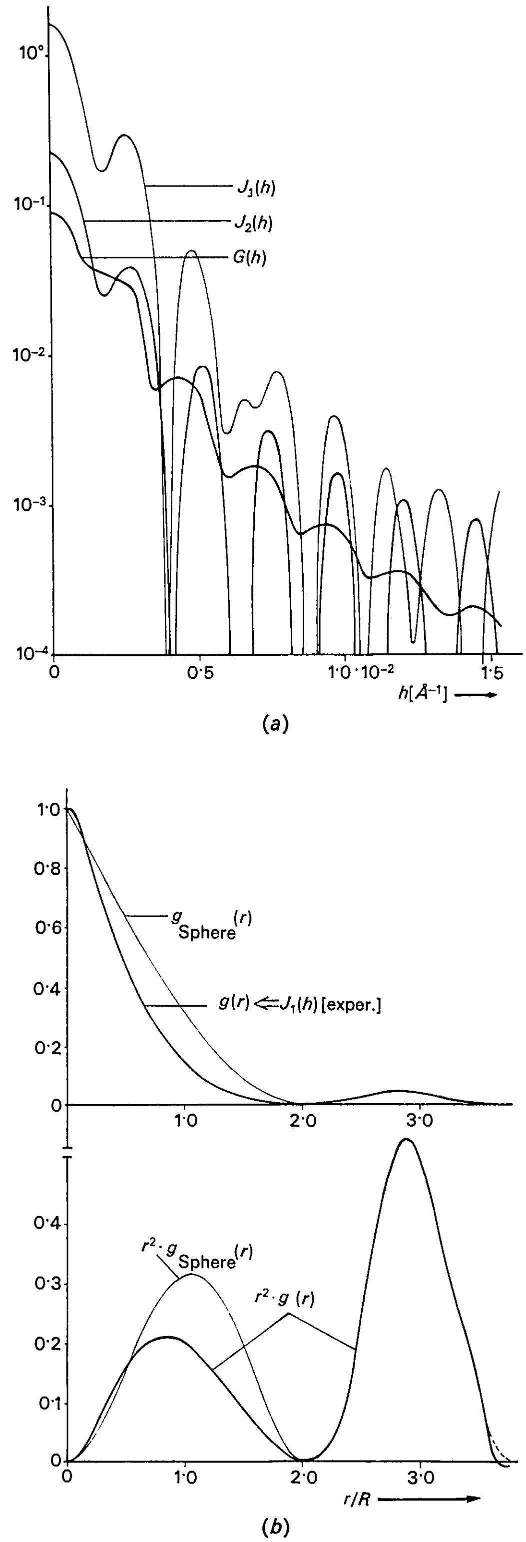

Fig. 2. X-ray small angle scattering of latex (after Bonse & Hart): (*a*) slit height corrections with $i_H(u)$=const, $|u|\le u_M$. $J_1(h)$: $u_M=1{\cdot}63\times10^{-2}$ Å^{-1}; $J_2(h)$: $u_M=2{\cdot}45\times10^{-2}$ Å^{-1}; (*b*) correlation function for a sphere, and $g(\mathbf{r})$ calculated from $J_1(h)$ with an interparticle effect present.

tion slits, and of the distortion effect caused by non-monochromatic radiation. These smearing effects can be corrected in a general and quantitative manner that is properly matched to the accuracy of the measurements. The methods lead to simple recurrence formulae, thus reducing calculations to a coefficient algebra easy to manipulate with digital computers. Error propagation may be discussed within the framework of the formalism of orthonormal functions.

The experimental scattering distributions are represented by discrete expansion coefficients in proper accord with the functional character of these distributions. Therefore this Hermite function formalism might prove useful in problems beyond the mere correction of errors, such as problems of optimizing small angle scattering experiments (Monahan & Langsdorf, 1965), and lead to a valuable means of information processing in this field.

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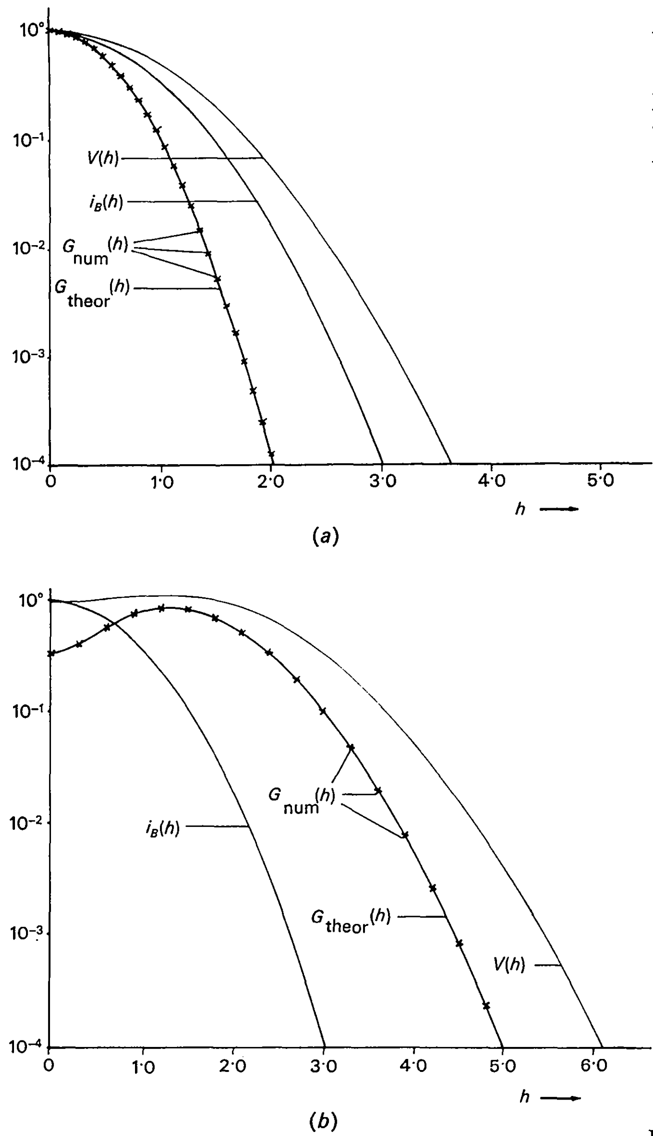

Fig. 3. Slit width correction with weighting function $i_B(h)=\exp(-h^2)$: (a) $G_{theor}(h)=\exp(-h^2/0{\cdot}44)$; (b) $G_{theor}(h)=(\frac{1}{3}+h^2)\exp(-h^2/2)$.

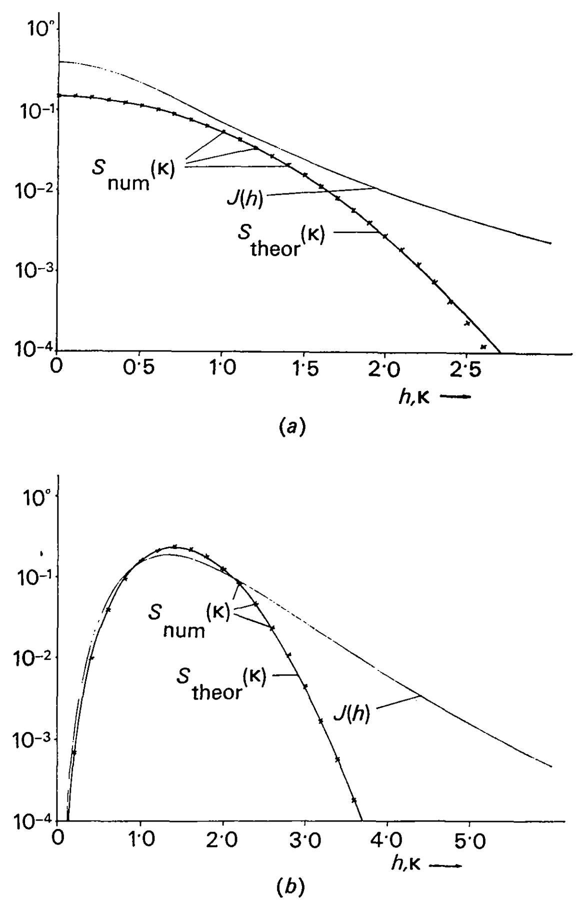

Fig. 4. Correction of function types $S_{theor}(x)=C\,.\,x^{2n}\exp(-x^2/b^2)$ for polychromatic distortion, with $z(k)=z_0\,.\,k^{m-2}\exp(-A^2k^2)$: (a) $n=0$, $b=1$, $m=5$, $A^2=0{\cdot}75$; (b) $n=2$, $b=1$, $m=9$, $A^2=0{\cdot}35$.

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Correction for Preferred Orientation of Plate-like Particles in Diffractometric Powder Analysis

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A major problem of quantitative powder diffraction analysis is the tendency of many samples to be preferentially oriented. The approach proposed here is to work with easily prepared, preferentially oriented flat samples, whose orientation can be characterized in quantitative terms. Once the orientation is known, the observed intensities may be corrected for the effects of orientation. Although the approach is general, correction factors are developed and experimental results are presented only for the most common mode of preferred orientation, as exhibited by plate-like particles.

Introduction

Any sample assemblage of morphologically anisotropic powder-sized particles tends to be preferentially oriented. To overcome the effects of preferred orientation, several techniques of sample preparation have been worked out which are supposed to result in randomly oriented samples (Byström-Asklund, 1966; Niskanen, 1964). No technique can guarantee ideally random orientation, and it is the uncertainty regarding the degree of randomness achieved which lowers the value of these techniques. Other techniques are attempts to derive the intensity of an equivalent, randomly oriented sample from the diffraction data of the preferentially oriented sample. Randomizing diffraction data from polymers showing certain types of preferred orientation has been attempted by employing specialized sample holders that spin the specimen, by weighting each quantum of the line profile by a certain function, and by integrating over the total angle intercepted (Desper & Stein, 1967). The tedium of the computational work can be almost eliminated by the use of an electronic device which combines the output of a pulse height analyzer with that of a function generator before integrating the modified signal (Ruland & Dewaelheyns, 1967). The aim of these techniques is to obtain meaningful intensity readings by averaging the diffraction data. The approach suggested here is to prepare preferentially oriented specimens and to determine the specific distribution function which characterizes the orientation. The effects of preferred orientation may then be cancelled out by correcting the observed intensities for the various reflections.

Wherever there is a finite probability that particles will assume a certain position, a normal distribution must result. In practice, the conditions for normal distributions are met by any aggregate of morphologically anisotropic particles whose tendency toward preferred orientation has not been interfered with. Therefore, the preferred orientation of powdered samples is best dealt with in terms of the normal distribution of radii of probability. We may characterize the orientation of a crystallite by the position of the perpendicular to a given crystallographic plane. The lengths of the radii of probability, drawn from a common origin, are proportional to the number of particles in the given direction, and therefore are also related to the observed intensities. The spatial distribution of intensities representing preferred orientation of platelets, for example, is cylindrically symmetrical and has a plane of symmetry perpendicular to the major direction or the longest radius. In this case, the distribution function