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A Theory for the Evaluation of Small-Angle Scattering Diagrams of Quasi Radially Symmetric Particles Considering Polydispersity and Deviations from Radial Symmetry

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Abstract

A general theory has been developed describing the scattering intensity of a polydisperse dilute ensemble of particles. These particles are assumed to be mainly radially symmetric. Deviations from radial symmetry are treated quantitatively using an expansion of the electron density in terms of multipole components. The particle radii are assumed to have a Gaussian-like distribution. The electron density of the particle core is allowed to be different from that of the solvent. As a practical application of this theory a Fortran 77 program was written which determines the radial electron density profile, the standard deviation of the radii, and additional parameters describing the deviations from spherical symmetry directly from the measured intensity.

I. Introduction

Theoretical expressions for the small-angle scattering of polydisperse membrane vesicles were given by Weick, Hosemann, Pape & Menke (1974) and Moody (1975).

Moody's theory is exact in the case of polydisperse ensembles with electron density of the particle core being equal to that of the solvent. The theory given by Weick *et al.* is an approximation of that given by Moody. Only Weick *et al.* give a concrete representation of the model electron density and the statistical function describing radius variations. This concrete representation is, however, essential for a practical application of the theory to evaluate scattering diagrams. Both theories do not include deviations from spherical symmetry.

In this paper a general theory is developed taking into account polydispersity and electron density difference between particle core and solvent, as well as non-radially-symmetric parts of the particle structure. The contributions of the non-radially-symmetric parts are quantitatively estimated, using an expansion of the electron density in terms of spherical harmonics, which was introduced by Stuhrmann (1970) to describe arbitrary one-particle scattering functions. In contrast to Stuhrmann's theory it is necessary for our theory, dealing with ensembles of particles, to consider effects of polydispersity on the multipole components.

Possible applications of our theory are more precise evaluations of scattering diagrams of lipoproteins, small membrane vesicles, and recombined lipoprotein particles.

II. Basic definitions and assumptions

\mathbf{b} is the scattering vector in reciprocal space, $b = 2 \sin(\theta)/\lambda$ (θ half scattering angle, λ wavelength); \mathbf{x} is the coordinate in real space; \mathcal{F} denotes the Fourier transform

$$\mathcal{F}[f(\mathbf{x})] = \int d^3x f(\mathbf{x}) \exp(-2\pi i \mathbf{b} \cdot \mathbf{x}); \quad (1)$$

the symbol \mathcal{L} denotes the convolution square

$$\mathcal{L} \frac{f}{g} = f(\mathbf{x}) * f^{-}(\mathbf{x}), \quad (2)$$

where the convolution operation $*$ is defined by

$$f(\mathbf{x}) * g(\mathbf{x}) = \int d^3y f(\mathbf{y}) g(\mathbf{x} - \mathbf{y}) \quad (3)$$

and f^{-} denotes $f(-\mathbf{x})$.

In the following calculations several basic assumptions are made

(a) The theoretical intensity $I(\mathbf{b})$ differs from the actual measurable intensity $I_{\text{exp}}(\mathbf{b})$ only by a constant factor, because the scattering factor of an electron f_e^2 and the polarization factor f_θ^2 are constant in the small-angle region (Guinier & Fournet, 1955).

(b) The target is assumed to be an infinitely dilute solution of particles, *i.e.* we have to calculate the scattering intensity of each particle and take the incoherent average over all orientations and particle sizes.

III. General approach for calculating one-particle scattering

A useful relationship connecting scattering intensity $I(\mathbf{b})$ and electron density $\rho(\mathbf{x})$ of a single arbitrary particle was given by Stuhrmann (1970). He uses an expansion of $\rho(\mathbf{x})$ in terms of spherical harmonics

$$\rho(\mathbf{x}) = \sum_{l=0}^{\infty} \sum_{m=-l}^l \rho_{lm}(r) Y_{lm}(\theta, \varphi) \quad (4)$$

and obtains as a final result, after averaging over all orientations of $\rho(\mathbf{x})$,

$$I(b) = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^l \left| \int_0^{\infty} \rho_{lm}(r) j_l(2\pi br) r^2 dr \right|^2, \quad (5)$$

where j_l denotes the spherical Bessel function of order l . For details see Stuhrmann & Miller (1978).

The main advantage of relationship (5) between $\rho(\mathbf{x})$ and $I(\mathbf{b})$ is the fact that there are no interference terms between different multipole components.

IV. Multipole term

The monopole term, which we assume to be the most important part of the particle structure, is given by

$$I(b) = 4/b^2 \left[\int_0^{\infty} \rho_r(r) r \sin(2\pi br) dr \right]^2, \quad (6)$$

which is obtained from (5) by substituting $j_0(z) = \sin(z)/z$ and $\rho_r(r) = \rho_{00}/(4\pi)^{1/2}$.

Equation (6) leads us to introduce an antisymmetric function $g(r)$ defined from $-\infty$ to $+\infty$:

$$g(r) = \begin{cases} r\rho_r(r) & r \geq 0 \\ r\rho_r(-r) & r < 0. \end{cases} \quad (7)$$

Using $g(r)$ we can write [$F(b)$: scattering amplitude]

$$b^2 I(b) = |\mathcal{F}g(r)|^2 \quad \text{or} \quad bF(b) = \mathcal{F}g(r). \quad (8)$$

If we apply the convolution theorem to the upper equation, we arrive at the following one-dimensional relationships between the functions $\rho_r(r)$ and $I(b)$.

$$\begin{array}{ccccc} & & | & | & \\ & & \downarrow & \downarrow & \\ I(b) & \longleftrightarrow & b^2 I(b) & \longleftarrow & bF(b) \\ & & \downarrow \mathcal{F} & & \downarrow \mathcal{F} \\ & & \rho(r) & \xleftarrow{\mathcal{L}} & g(r) & \longleftrightarrow & \rho_r(r) \end{array} \quad (9)$$

For arbitrary functions a general solution of these equations is impossible, but it can be shown that a solution is possible introducing two conditions (Hosemann & Bagchi, 1962):

(1) $g(r)$ has to be a band-limited function

$$g(r) = \begin{cases} \text{if } x < -R_s; \\ 0 \\ \text{if } x > R_s \end{cases} \quad (10)$$

(2) $g(r)$ has to be a symmetric or antisymmetric function, and consequently transforms to a pure real or imaginary function with only two possible phases.

V. Phase problem, unique solution

If one applies the sampling theorem (see Bracewell, 1965) to (8), one obtains an important insight into the information contained in the scattering intensity $I(b)$: $|bF(b)|$ can be reconstructed from a limited number of equally spaced sampling points of $bF(b)$ (McIntosh & Worthington, 1974).

$$|bF(b)| = \left\| \sum_{k=0}^{\infty} s_k \left| \frac{k}{L} F(k/L) \right| \left| \frac{\sin(\pi L b - \pi k)}{(\pi L b - \pi k)} \right| \right\|. \quad (11)$$

$1/L$ denotes the sampling distance, with L being equal to or larger than the maximum extension of $g(r)$. Equation (11) holds for arbitrary phases s_k only at the sampling points $b = k/L$. Between these sampling points (11) is only valid for the true phase combination

and one with + and - interchanged. This means that the phase information is contained in the course of $F(b)$ between the sampling points.

The solution $g(r)$ is given by a Fourier series

$$g(r) = \frac{1}{L} \sum_{k=0} s_k \left| \frac{k}{L} F\left(\frac{k}{L}\right) \right| \exp(2\pi i r k / L) \quad (12)$$

whose coefficients $s_k |bF(b)|$ with $b = k/L$ are exactly the sampling point of $F(b)$.

A deconvolution of $p(r)$ is possible on the same conditions that were necessary for solving (8). The problem of deconvolution (Hosemann & Bagchi, 1962; Pape, 1974; Glatter, 1981) will not be treated further in this article. We intend only to give a more precise statement about the phase information contained in $I(b)$.

Since the extension of $p(r)$ is twice that of $g(r)$, the sampling distance for sampling $I(b)$ has to be half that for sampling $F(b)$. This means that the phase information is contained not in the total course of $|F(b)|$ between two sampling points k/L , but only in odd-numbered sampling points $(2k + 1)/(2L)$ of $I(b)$.

VI. Polydisperse ensemble of radially symmetric particles

The methods for solving (9) given in the preceding section are valid only for monodisperse systems. We will now develop a model for $\rho_r(r)$ similar to that described by Welte & Kreutz (1979) for the case of lamellar systems, which makes it possible to give an equation for the scattering intensity of a polydisperse ensemble of particles. Since the scattering intensity of a partial multipole component can be calculated independently from all others (equation 5), we will start with the most important part, the monopole component.

When assuming infinitely dilute systems the scattering intensity $I(b)$ of an ensemble with distribution function h is given as an incoherent average of the individual scattering intensities $I_s(b, R_s)$ of one particle with radius R_s .

$$I(b) = \int_{-\infty}^{+\infty} h(R_s) I_s(b, R_s) dR_s. \quad (13)$$

Since Fourier transformation and average can be interchanged, averaging intensities is equivalent to averaging autocorrelation functions $p_s(r)$ in real space.

$$I(b) = \mathcal{F} p(r) = \mathcal{F} \left[\int_{-\infty}^{+\infty} h(R_s) p_s(r, R_s) dR_s \right]. \quad (14)$$

In the following we will calculate the scattering intensity of polydisperse radially symmetric particles according to (14).

To be able to describe particles of different sizes we compose a function $\rho_s(r) = g_s(r)/r$ from three parts (Fig. 1): the radial electron density $\rho_m^-(r)$ of a particle with mean radius R_m , its mirror image $\rho_m^+(r)$, and a rectangle function $z(x, r)$ to correct resulting gaps or overlaps of ρ_m and ρ_m^- inside the core of the particle, for the case of larger or smaller vesicles.

Mathematically this model can be described by (15).

$$g_s(r) = r \{ \rho_m(r + \Delta R) + \rho_m^-(r - \Delta R) + h_i \sigma_s z(|2\Delta R|, r) \} \quad (15)$$

with the following abbreviations used:

$$z(x, r) = \begin{cases} 0 & |r| > x/2 \\ 1 & |r| \leq x/2 \end{cases}$$

$$\Delta R = R_s - R_m$$

$$\sigma_s = \begin{cases} +1 & R_s > R_m \\ -1 & R_s < R_m \end{cases}$$

$$h_i = \rho_m(r = 0).$$

The resulting expression for $I(b)$ after calculating $p_s(r)$, averaging, and Fourier transform† is given in (16).

$$\begin{aligned} b^2 I(b) &= 2|Ka - \langle \Delta R \rangle Ro|^2 + 2\sigma_R^2 |Ro|^2 \\ &\quad - 2 \operatorname{Re} \{ Ka^2 H^*(b) \} \\ &\quad + 2 \operatorname{Re} \left\{ RoKa \frac{i}{2\pi} H^{*'}(b) \right\} \\ &\quad + \frac{1}{2} \operatorname{Re} \left\{ Ro^2 \frac{1}{4\pi^2} H^{*''}(b) \right\} \\ &\quad - 4h_i \operatorname{Re}(Ka) \operatorname{ZPIS} + 4h_i i \operatorname{Im}(Ro) \operatorname{ZPIA} \\ &\quad + h_i^2 \operatorname{ZQIS}, \end{aligned} \quad (16)$$

† Details of the calculations as well as numerical tests and a description of the program have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38020 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

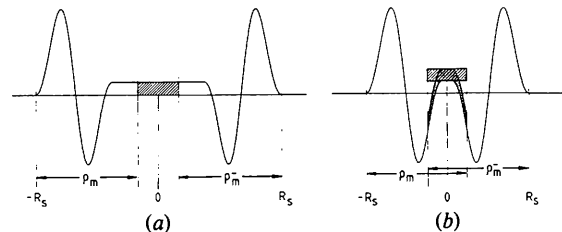


Fig. 1. (a) The two halves ρ_m and ρ_m^- were shifted apart from each other to obtain the desired radius $R_s > R_m$. The resulting gap is filled by adding a rectangle function. (b) For the case of $R_s < R_m$ the two halves ρ_m and ρ_m^- are shifted towards each other. The resulting overlap is corrected by subtracting a rectangle function.

with the symbols

$$Ro(b) = \mathcal{F}\rho_m(r)$$

$$Ka(b) = \mathcal{F}[r\rho_m(r)]$$

$$H^*(b) = \mathcal{F}h(-r)$$

' denotes derivation

σ_R standard deviation of radii

ZPIS } 'rectangle terms' resulting from convolution
 ZPIA } products of $z(x,r)$
 ZQIS }

Re real part

Im imaginary part.

Moody's (1975) equation for $I(b)$ is obtained from (16) by the approximation $h_i = 0$. This means that the electron density inside the core of the particle has to be the same as that of the solvent.

To be able to use (16) for the determination of electron density profiles it is necessary to introduce assumptions concerning the functions ρ_m and h :

(a) $\rho(r) = \rho_m^-(r) + \rho_m(r)$ can be described by a Fourier series. Since $\rho(r)$ is a symmetric function a cos series is sufficient. The function $\rho_m(r)$ is the left part of this series:

$$\rho_m(r) = \begin{cases} \sum_{k=0}^{\infty} c_k \cos(2\pi k/Lr) & 0 \geq r \geq -R_m \\ 0 & \text{elsewhere.} \end{cases} \quad (17)$$

(b) The radius variations of the particles are described by a Gaussian statistical function with a mean diameter $L = 2R_m$, actual diameter $L_s = 2R_s$ and standard deviation σ ($\sigma = 2\sigma_R$).

$$h(R_s) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left[-\frac{(2R_s - 2R_m)^2}{2\sigma^2}\right]. \quad (18)$$

$\langle \Delta R \rangle$ is zero for this choice of h .

(c) According to the sampling theorem it is sufficient to calculate the Fourier transform (equation 14) only at discrete sampling points. Using the approximation that $h = 0$ for $L_s - L > 3\sigma$ we need sampling distances of at least $1/(2L + 6\sigma)$, since $2L + 6\sigma$ is the maximal extension of $p(r)$. For simplicity we use sampling distances of $1/(NL)$, which are sufficient for σ up to 66%, using $N = 4$.

With these assumptions it is possible to calculate the terms of (16) explicitly. They are given in the Supplementary Publication.

(1) Scattering intensity for the case of small polydispersity

In the case of monodisperse particles only the term proportional to $|Ka|^2$ ($\langle \Delta R \rangle = 0$) and $\text{Re}(Ka^2)H(b)$ contribute to (16), since all other terms vanish for $\sigma = 0$. It can be expected that also in the case of polydispersity with small σ these two functions domin-

ate the scattering intensity. As shown by Fig. 2 the typical scattering intensity of radially symmetric particles originates from the combination of the two quite different functions $|Ka|^2$ and $\text{Re}(Ka^2)$. The latter is a function oscillating around zero, while the absolute square $|Ka|^2$ is a decreasing function, showing no oscillations. All other terms contribute only small corrections. The influence of the statistical function can easily be discussed, since $|Ka|^2$ is not influenced by polydispersity, while the oscillating term $\text{Re}(Ka^2)$ is multiplied by a factor $H(b) = \exp(-2\pi^2\sigma^2b^2)$ which means that its amplitude decreases more and more for increasing values of σ or b . This corresponds to the experimentally observed facts that with increasing polydispersity the number of side maxima decreases, and that the minima of the scattering intensity no longer reach zero.

It has to be emphasized that not only the amplitude and number of side maxima are affected by polydispersity, but also a shift in the position of the side maxima to smaller b values occurs. This shift results from the multiplication of the monotonely decreasing Gaussian (Fig. 4) with the oscillating term. As can be seen in Fig. 3 this shift is clearly visible for a relatively small σ of 4%. Consequently, an interpretation of scattering intensities of polydisperse samples using monodisperse theory leads, apart from other effects, to artificially increased particle radii.

(2) Scattering intensity for larger polydispersity

In the case of larger σ values three additional terms proportional to $\text{Re}(Ro^2)H''$, $\sigma^2|Ro|^2$, and $RoKaH'$ have to be considered, since all three terms contain a factor σ^2 and σ^4 . The statistical functions appearing in these terms are shown in Fig. 4. As can be seen in Fig.

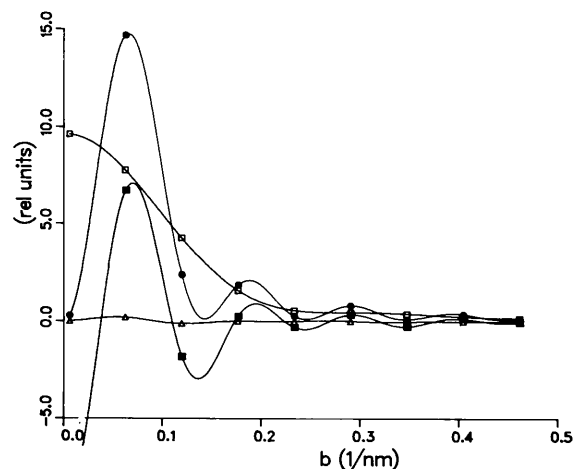


Fig. 2. Total scattering function Ib^2 (●) and its partial terms $2|Ka|^2$ (□), $-2 \text{Re}(Ka^2)H$ (■), and the sum of the remaining terms (△) in the case of a sphere ($c_0 = 1$, all other $c_k = 0$) and a standard deviation of radii of $\sigma_R = 4\%$.

4 the functions $\text{Re}(Ro^2)H''$ and $\sigma^2|Ro|^2$ show a similar behaviour to $\text{Re}(Ka^2)H$ and $|Ka|^2$. An additional oscillating term is $RoKaH'$. The 'rectangle terms' produce only small contributions in the case of a statistical function with $\langle \Delta R \rangle = 0$. Important contributions of these terms can be expected for asymmetric statistic functions with $\langle \Delta R \rangle > 0$, and high electron density differences between particle core and solvent.

With $\sigma \rightarrow \infty$ the situation becomes easy again. All terms containing $H(b)$ or a derivation thereof vanish for

$b > 0$. The only remaining term is $\sigma^2|Ro|^2$. This case is realized, for example, in the case of big membrane vesicles with extreme radius variations. The p function now consists only of the convolution square of the electron density profile of a single membrane. The scattering curve equals that of a flat membrane stack showing the same distance distribution.

(3) Information content of $I(b)$

Two principal pieces of information can be obtained from $I(b)$: firstly the radial electron density profile, and secondly the amount of polydispersity.

(a) Radial electron density profile $\rho_r(r)$. It was shown that in the case of monodisperse solutions the complete information regarding $\rho_r(r)$ (apart from a factor -1) is present in $I(b)$. With polydisperse

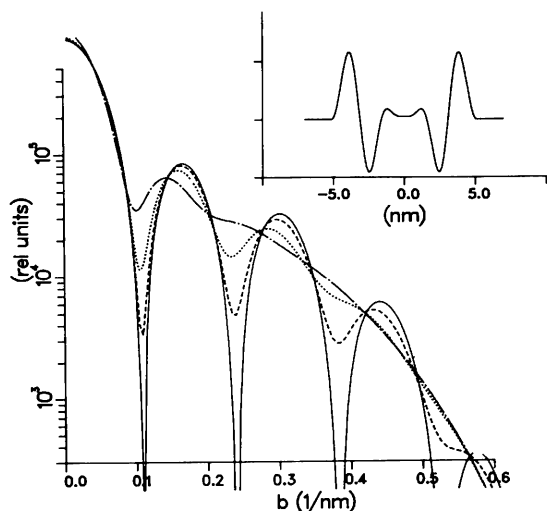


Fig. 3. Scattering intensities calculated for $\sigma_R = 0\%$ (—), 4% (---), 8% (···), and 16% (—·). Upper right: $\rho_m + \rho_m^-$ used for this model calculation.

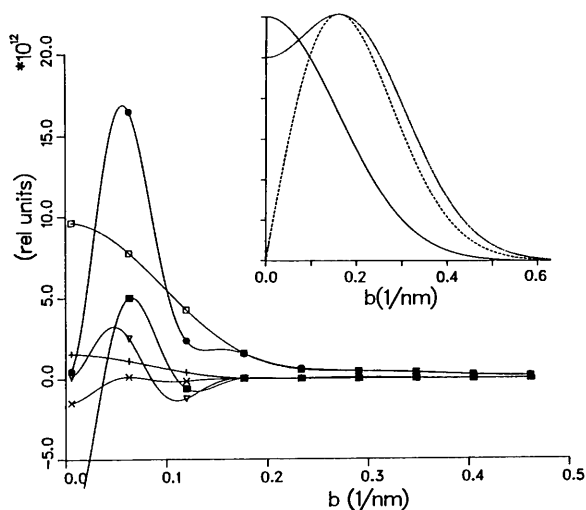
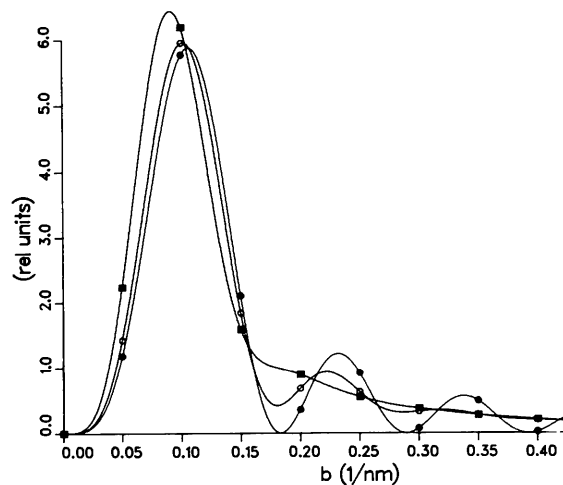
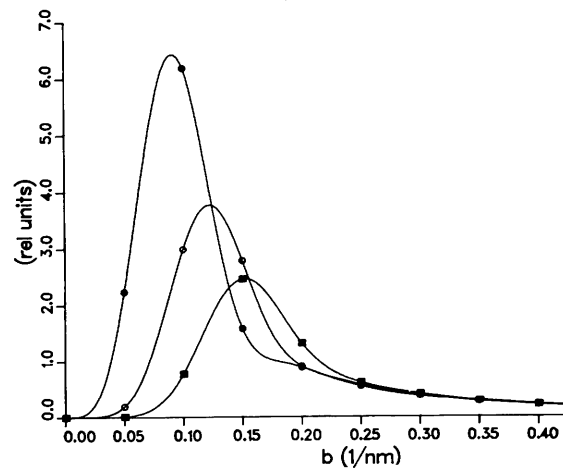


Fig. 4. Total scattering function Ib^2 (●) and its partial terms $2|Ka|^2$ (□), $-2 \text{Re}(Ka^2)H$ (■), $2\sigma_R^2|Ro|^2$ (+), $1/(4\pi^2) \times \text{Re}(Ro^2)H''$ (×), and $2 \text{Re}[RoKa i/(2\pi)H']$ (∇) in the case of a sphere ($c_0 = 1$, all other $c_k = 0$) and a standard deviation of radii of $\sigma_R = 20\%$. Upper right: Statistical functions H (—), $b\sigma^2 H$ (---), and $(-\sigma^2 + 4\pi^2 b^2 \sigma^2)H$ (···) for $\sigma_R = 1 \text{ nm}$. All normalized to the same maximum amplitude.



(a)



(b)

Fig. 5. (a) Effect of polydispersity on the scattering intensity of a quadrupole ($l = 2$). $\sigma = 0\%$ (●), $\sigma = 10\%$ (○), and $\sigma = 20\%$ (■). (b) Scattering intensities of three different multipoles all having the same polydispersity of $\sigma = 20\%$. $l = 2$ (●), $l = 3$ (○), and $l = 4$ (■).

ensembles this information is accessible only up to a certain amount of σ . To show this we first discuss $\sigma \rightarrow \infty$.

In this extreme case only the information of $\sigma^2 |R\sigma|^2$ remains, which is the convolution square of $\rho_m(r)$. Since in general $\rho_m(r)$ shows no centre of symmetry a deconvolution is not possible, and therefore $\rho_r(r)$ cannot be retrieved.

To obtain a unique solution for $\rho_r(r)$ it must be required that $H(b)$ does not decrease too fast, to allow contributions of the oscillating terms, which are obviously essential for phase determination, to be still present in $I(b)$. This means that at least one or two side maxima should be measured with a reasonable signal-to-noise ratio.

(b) *Size distribution.* Since the statistical function $H(b)$ acts only on the oscillating terms, it is obvious that its σ can only be determined if the oscillating terms are visible, which is the same condition as in (a).

VII. Polydisperse non-radially symmetric particles

In the case of non-radially symmetric particles $I(b)$ has to be computed as a sum of different multipole scattering intensities (equation 5). Because of polydispersity each of these multipole intensities has to be calculated, like the monopole intensity, as an incoherent average:

$$I_{im} = \int_{-\infty}^{+\infty} h_{im}(R) I_{im}^s(b, R) dR, \quad (19)$$

with the scattering intensity of a single multipole component being

$$I_{im}^s = 4\pi \left| \int_0^{\infty} \rho_{im}(r) j_l(2\pi br) r^2 dr \right|^2. \quad (20)$$

As in the radially symmetric case model assumptions concerning the functions h_{im} and ρ_{im} have to be introduced.

To give an idea of the form of these polydisperse multipole scattering intensities Fig. 5 shows several

intensities for the simple case of $\rho_{im} = \delta(r - R)$ and $h_{im}(R) = \exp[-(R - R_m)^2/(2\sigma^2)]$. The average (equation 19) was computed numerically. It is obvious that a treatment of each multipole component, as exact as that in the radially symmetric case, leads to a drastically increased number of parameters to be determined.

A useful application of this theory requires structures either with one multipole component being dominant, and only a few others necessary for describing the particle structure, or with structures having radial dependencies $\rho_{im}(r)$ that are easily described.

In the Supplementary Publication a computer program is outlined, which is suitable for particles which are mainly radially symmetric. In addition, the results of numerical tests are given.

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