Application of orthogonal polynomials to estimation of scattering coefficients of polydisperse randomly oriented spheroidal particles

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Orthogonal polynomials are used for few-parameter estimation of extinction, scattering and absorption coefficients of polydispersions of spherical and randomly oriented spheroidal particles. The estimation is based on equivalence (relation of equivalence is set by equality of the moments of distribution) of polydispersions of randomly oriented spheroidal particles and discrete ensemble of spherical particles. Quadrature formulae of Gaussian type, accurate to $(2n - 1)$ power inclusive are constructed and their physical interpretation is discussed. The error of the quadrature formulae is estimated, the results are compared with the numerical results of rigorous theory for polydispersions of randomly oriented spheroidal particles.

Introduction

Construction of mathematical models is based on mathematical notion of ratio of equivalency, or “equality.”[1] Parameters of mathematical models coincide with some basic parameters of an actual object. The ratio of equality of the model parameters determines the ratio of equivalency, and “divides” all mathematical objects into non-crossing classes of equivalency. From the standpoint of the model, the objects are indistinguishable within the limits of one class, and any representative characterizes the class as a whole and can be selected as the simplest for further investigation.

Construction of few-parameter models for estimation of the scattering coefficients (cross sections) of an isotropic ensemble of spheroidal particles presented in this paper, which logically continues and generalizes the approach from Ref. 2, is based on the use of orthogonal polynomials.[3]

1. Polydisperse ensembles of spherical particles

Let us consider an elementary scattering volume containing a polydisperse ensemble of spherical particles with the known size distribution density function $\rho(r)$. The extinction, scattering and absorption coefficients have the form

$$\langle C(m_{\rm r}, \lambda)\rangle = \int\limits_{r_1}^{r_2} C(m_{\rm r}, \lambda, r)\, \rho(r)\, {\rm d}r, \qquad (1)$$

where $[r_1, r_2]$ is the range of variations of the dimensional parameters; λ is the wavelength of the incident radiation, $m_{\rm r}$ is the relative refractive index. Let us suppose then that the refractive index and the wavelength be invariable and omit them.

The integral (1) can be estimated using the quadrature formulas of the Gaussian type,[3] where the weight function is the distribution density function $\rho(r)$. The quadrature formulas of the Gaussian type are the formulas of the following form:

$$\int\limits_a^b f(x)\, \rho(x)\, {\rm d}x \simeq \sum_{i=1}^{n} \lambda_i f(x_i), \qquad (2)$$

where the weight coefficients λ_i and the nodes x_i $(i = 1, 2,\dots, n)$ are chosen so that formula (2) is accurate for an arbitrary polynomial of the power $(2n - 1)$ inclusive.

The nodes x_i $(i = 1, 2,\dots, n)$ are the roots of the polynomial $p_n(x)$ of the system of orthogonal polynomials on the interval (a, b) of the weight $\rho(x)$. Using the properties of the orthogonal polynomials, we can obtain an explicit formula[3]:

$$p_n(x) = A_n \begin{bmatrix} C_0 & C_1 & \dots & C_n \\ C_1 & C_2 & \dots & C_{n+1} \\ . & . & . & . \\ C_{n-1} & C_n & \dots & C_{2n-1} \\ 1 & x & \dots & x^n \end{bmatrix}, \qquad (3)$$

where A_n is the normalizing constant,

$$C_k = \int\limits_a^b x^k\, \rho(x)\, {\rm d}x.$$

The coefficients λ_i $(i = 1, 2,\dots, n)$ are determined using the Darbu–Christoffel formula,[3] or at the known x_i $(i = 1, 2,\dots,n)$ as a solution of the system of linear equations under condition that formula (2) is accurate

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for an arbitrary set of n linearly independent polynomials of the power $(2n - 1)$ inclusive.

The estimate of the integral (1) using Gaussian quadrature formula (2) has the following physical interpretation: a discrete ensemble of spherical particles, the size spectrum of which coincides with the nodes of the quadrature formula is put in correspondence with a polydisperse ensemble of spherical particles. The weighting factors are considered as the concentration coefficients, and so the discrete ensemble has the moments of the distribution equal to that of the initial ensemble up to $(2n - 1)$ inclusive. Thus, these ensembles of particles belong to the same class of equivalency, where the ratio of equivalency is set by the equality of the moments of the distributions.

2. Polydisperse ensembles of randomly oriented spheroidal particles

Estimation of the scattering coefficients of randomly oriented monodisperse ensembles of spheroidal particles is based on the optical equivalency (in the Rayleigh–Gans–Debye approximation) to the polydisperse ensemble of spherical particles with the corresponding weighting function $\rho(a, b, r)$ (see, e.g., Ref. 2), and, thus, is reduced to analogous problem for a polydisperse ensemble of spherical particles. The function of the joint distribution of a, b, and r in the case of polydisperse ensemble of randomly oriented spheroids with the size distribution density function $f(a, b)$ has the form of the convolution[4]:

$$\rho_0(a, b, r) = f(a, b) * \rho(a, b, r). \quad (4)$$

Here a and b are the spheroid semi-axes. The weighting function of the equivalent polydisperse ensemble of spherical particles $\rho(r)$ is determined from integration of expression (4) over the range of a and b variation.

3. Calculated results

The algorithm for few-parameter estimation of the extinction, scattering and absorption coefficients of polydisperse ensembles of randomly oriented spheroidal particles includes the following steps:

1) determination of the moments, C_k, of the distribution for the weighting function $\rho(r)$ of the equivalent polydisperse ensemble of spherical particles;

2) determination of the roots (x_i, $i = 1, 2, \ldots, n$) of the polynomial $p_n(x)$ (3) and the weighting factors λ_i, $i = 1, 2, \ldots, n$;

3) calculation of the scattering coefficient of the discrete ensemble of spherical particles by formula (2).

Table gives the calculated results (accurate to the factor k^{-2}, where k is the wave number) on the extinction, scattering, and absorption coefficients of polydisperse ensemble of randomly oriented oblate spheroids with the distribution density function

$$f(a, b) = f(\varepsilon b, b) = \frac{2b_{\min}^2\, b_{\max}^2}{\varepsilon(b_{\max} - b_{\min})^2\,(b_{\max} + b_{\min})}\, b^{-3},$$

$$b_{\min} \le b \le b_{\max}, \quad (5)$$

where ε is the shape parameter equal to the semi-axis ratio and the relative refractive indices m_r corresponding to biological and terrigenic components of the oceanic suspension and aerosols of mineral origin in the visible wavelength range. The following methods were used: the exact theory (T-matrix method[5]) and the proposed few-parameter estimation. In all considered cases $\varepsilon = 3$.

Table

Method	C_{ext}	C_{scat}	C_{abs}
	$m_r = 1.05 + i0.0001$, $kb_{\min} = 1$, $kb_{\max} = 10$		
T-matrix	23.83	23.68	0.149
$n = 3$	23.72	23.56	0.148
$n = 4$	23.65	23.51	0.148
	$m_r = 1.15$, $kb_{\min} = 1$, $kb_{\max} = 10$		
T-matrix	110.3	110.3	0
$n = 3$	102.3	102.3	0
$n = 4$	111.0	111.0	0
	$m_r = 1.5 + i0.0001$, $kb_{\min} = 0.1$, $kb_{\max} = 5$		
T-matrix	1.662	1.661	0.00134
$n = 3$	1.367	1.366	0.00143
$n = 4$	1.545	1.544	0.00142
$n = 5$	1.737	1.736	0.00131
$n = 7$	1.667	1.666	0.00128

Conclusion

The few-parameter models constructed are optimal for estimation of the scattering coefficients of polydisperse ensembles of spherical particles using the number of nodes of the quadrature formula, which has quite obvious physical interpretation. An isotropic ensemble of spheroidal particles and the constructed equivalent discrete ensemble of spherical particles have the same mean volume and geometric cross section.

References

1. B. Van der Varden, *Modern Algebra*. Part 1 (Gostekhizdat, Moscow, 1947).
2. L.E. Paramonov, Atmos. Oceanic Opt. **7**, No. 8, 613–618 (1994).
3. A.F. Nikiforov and V.B. Uvarov, *Special Functions of Mathematical Physics* (Nauka, Moscow, 1984), 344 pp.
4. V.S. Vladimirov, *Equations of Mathematical Physics* (Nauka, Moscow, 1971), 512 pp.
5. P.C. Waterman, Phys. Rev. D **3**, No. 4, 825–839 (1971).