Light scattering by randomly oriented axially symmetric particles

M. I. Mishchenko

Laboratory for Radiative Transfer Theory, The Main Astronomical Observatory of the Ukrainian Academy of Sciences, 252127 Kiev-127, Goloseevo, USSR

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Light scattering by ensembles of independently scattering, randomly oriented, axially symmetric particles is considered. The elements of the scattering matrices are expanded in (combinations of) generalized spherical functions; this is advantageous in computations of both single and multiple light scattering. Waterman's T-matrix approach is used to develop a rigorous analytical method to compute the corresponding expansion coefficients. The main advantage of this method is that the expansion coefficients are expressed directly in some basic quantities that depend on only the shape, morphology, and composition of the scattering axially symmetric particle; these quantities are the elements of the T matrix calculated with respect to the coordinate system with the z axis along the axis of particle symmetry. Thus the expansion coefficients are calculated without computing beforehand the elements of the scattering matrix for a large set of particle orientations and scattering angles, which minimizes the numerical calculations. Like the T-matrix approach itself, the method can be used in computations for homogeneous and composite isotropic particles of sizes not too large compared with a wavelength. Computational aspects of the method are discussed in detail, and some illustrative numerical results are reported for randomly oriented homogeneous dielectric spheroids and Chebyshev particles. Results of timing tests are presented; it is found that the method described is much faster than the commonly used method of numerical angle integrations.

1. INTRODUCTION

A medium frequently encountered in light scattering is an ensemble of independently scattering nonspherical particles in which all possible orientations of a single particle are equally probable. In theoretical calculations of single and multiple light scattering by such media, a useful and efficient approach is to expand the elements of the scattering matrix in a suitable complete set of orthogonal functions, namely, in generalized spherical functions.[1–5] There are at least two reasons in favor of this approach. First, if the corresponding expansion coefficients are known, then the elements of the scattering matrix can be accurately evaluated for a large set of scattering angles with a minimum expense of computer time. Thus extensive light-scattering tables become unnecessary, and no interpolation is required for calculation of the scattering matrix in intermediate points. Second, the expansion coefficients easily enable one to calculate Fourier components of the phase matrix appearing in the equation of transfer of polarized light in plane-parallel isotropic media. As a result, both theoretical and numerical solutions of the radiative transfer equation are greatly simplified.[6–23]

Two efficient analytical methods for calculating the expansion coefficients for homogeneous spherical particles have been proposed by Domke[24] and Bugaenko[25] (note that equations analogous to those of Domke have been independently derived by Oguchi[10]). They have taken into account that each term in the Mie series is a product of one of the functions π_n and τ_n, which depend only on the scattering angle, and one of the Mie coefficients a_n and b_n, which depend only on the size parameter and refractive index of the scattering particle. By using this particular structure of the Mie series, Domke and Bugaenko have analytically expressed the expansion coefficients directly in the Mie coefficients. Thus in both methods the expansion coefficients are calculated without computing preliminarily the elements of the scattering matrix for a representative set of scattering angles, which minimizes the numerical work. Moreover, these methods are numerically accurate in the following sense: if a computational parameter $n_{\max}$ has been chosen, the Mie coefficients a_n and b_n for $n \leq n_{\max}$ are assumed to be determined precisely, and the coefficients for $n > n_{\max}$ are assumed to vanish, then the accuracy of computing the corresponding expansion coefficients is limited only by round-off errors and does not depend on any additional computational parameter (e.g., the number of division points of a quadrature formula used in the method of numerical angle integrations[26]). Recently Domke's method was reconsidered and improved by de Rooij and van der Stap,[26] whereas Mishchenko[27] has pointed out that this method can be applied to arbitrary radially inhomogeneous spherical scatterers. Note that the same is true for Bugaenko's method as well.

The purpose of the present paper is to consider a more general type of scattering, namely, light scattering by randomly oriented nonspherical particles of revolution. As a mathematical and numerical basis, we use Waterman's T-matrix approach,[28–32] which seems to be the most powerful tool for solving light-scattering problems for homogeneous and composite axially symmetric particles of sizes not too large compared with a wavelength.[33–41] I demonstrate that, like the Mie theory, the T-matrix approach enables one to solve analytically the problem of calculating the expansion coefficients relevant to the scattering matrices averaged over the uniform orientation distribution of axially symmetric scatterers. More specifically, I show that, instead of computing numerically the average scattering properties of a particle ensemble by averaging results for scattering by a single particle with continuously varying orientation, one

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can express the expansion coefficients analytically in some basic quantities that depend only on the size, morphology, and composition of the scattering particle and do not depend on any angular variable. These basic quantities are the elements of the T-matrix of the axially symmetric scatterer calculated with respect to the coordinate system with the z axis along the axis of symmetry.

The plan of this paper is as follows. In Section 2, I briefly recapitulate basic definitions and equations relevant to the scattering of light by a single nonspherical particle and by an ensemble of randomly oriented particles. Two sets of Stokes parameters are used to describe the state of polarization of light, and the corresponding scattering matrices are expanded in (combinations of) generalized spherical functions. A review of the T-matrix formulas is given in Section 3. Section 4 is a crucial part of the paper and contains derivations of simple analytical expressions that can be used for efficient numerical computations of the expansion coefficients and the elements of the scattering matrices of ensembles of randomly oriented particles of revolution. In Section 5 I discuss computational aspects of the proposed method and present some illustrative numerical results for randomly oriented homogeneous dielectric spheroids and Chebyshev particles.[34] The principal results of the paper are discussed and summarized in Section 6.

2. SCATTERING MATRIX

To describe the scattering of polarized light in some scattering medium, we use a right-handed Cartesian-coordinate system B with orientation fixed in space, having its origin inside a single scattering particle (Subsection 2.A) or inside a small volume element (Subsection 2.D). In what follows, this coordinate system will be referred to as the laboratory reference frame.

The direction of a beam of light is specified by a unit vector $\hat{n} = (\theta, \varphi)$, where $\theta (0 \le \theta \le \pi)$ is a polar angle measured from the positive z axis and $\varphi (0 \le \varphi \le 2\pi)$ is an azimuth angle measured from the positive x axis in the clockwise sense, when one is looking in the direction of the positive z axis.

θ and φ components of the electric field $\mathbf{E}$ are denoted by subscripts 1 and 2, respectively. Thus the component $\mathbf{E}_1 = E_1\hat{\theta}$ is along the meridional plane (plane through the beam and the z axis), whereas the component $\mathbf{E}_2 = E_2\hat{\varphi}$ is perpendicular to this plane; here, $\hat{\theta}$ and $\hat{\varphi}$ are the corresponding unit vectors (note that $\hat{n} = \hat{\theta} \times \hat{\varphi}$).

A. Amplitude Scattering Matrix

Consider a plane electromagnetic wave

$$\mathbf{E}^i(\mathbf{r}) = (E_1{}^i\hat{\theta}_i + E_2{}^i\hat{\varphi}_i)\exp(ik\hat{n}_i\mathbf{r}), \tag{2.1}$$

incident upon a nonspherical particle; here, $k = 2\pi/\lambda$, and λ is a free-space wavelength. The time factor $\exp(-i\omega t)$ is assumed and is suppressed throughout the paper. In the far-field region ($kr \gg 1$), the scattered wave becomes spherical and is given by (cf. Refs. 42 and 43)

$$\mathbf{E}^s(\mathbf{r}) = E_1{}^s(r, \hat{n}_s)\hat{\theta}_s + E_2{}^s(r, \hat{n}_s)\hat{\varphi}_s, \qquad \hat{n}_s = \mathbf{r}/r,$$

$$\mathbf{E}^s(\mathbf{r}) \cdot \mathbf{r} = 0,$$

$$\begin{bmatrix} E_1{}^s \\ E_2{}^s \end{bmatrix} = \exp(ikr)/r\, \mathbf{S}(\hat{n}_s; \hat{n}_i) \begin{bmatrix} E_1{}^i \\ E_2{}^i \end{bmatrix}, \tag{2.2}$$

where $\mathbf{S}$ is a (2×2) amplitude scattering matrix. This matrix depends on (besides $\hat{n}_i$ and $\hat{n}_s$) the size, morphology, and composition of the scattering particle as well as on the particle's orientation with respect to the laboratory reference frame B.

Circular components of the electric field are defined by[4]

$$\begin{bmatrix} E_{+1} \\ E_{-1} \end{bmatrix} = 1/\sqrt{2} \begin{bmatrix} 1 & i \\ 1 & -i \end{bmatrix} \begin{bmatrix} E_1 \\ E_2 \end{bmatrix} = 1/\sqrt{2} \begin{bmatrix} E_1 + iE_2 \\ E_1 - iE_2 \end{bmatrix}. \tag{2.3}$$

We easily verify that the corresponding amplitude scattering matrix $\mathbf{C}$ is given by

$$\mathbf{C} = \begin{bmatrix} C_{+1+1} & C_{+1-1} \\ C_{-1+1} & C_{-1-1} \end{bmatrix} = \frac{1}{2} \begin{bmatrix} S_{11} - iS_{12} + iS_{21} + S_{22} & S_{11} + iS_{12} + iS_{21} - S_{22} \\ S_{11} - iS_{12} - iS_{21} - S_{22} & S_{11} + iS_{12} - iS_{21} + S_{22} \end{bmatrix}, \tag{2.4}$$

where the arguments $(\hat{n}_s; \hat{n}_i)$ are omitted for brevity.

B. Stokes Parameters

In this paper we use two sets of Stokes parameters of the incident plane wave and the scattered spherical wave defined as[4]

$$I = E_1E_1{}^* + E_2E_2{}^*, \tag{2.5a}$$

$$Q = E_1E_1{}^* - E_2E_2{}^*, \tag{2.5b}$$

$$U = -E_1E_2{}^* - E_2E_1{}^*, \tag{2.5c}$$

$$V = i(E_2E_1{}^* - E_1E_2{}^*) \tag{2.5d}$$

and

$$I_2 = E_{-1}E_{+1}{}^* = \tfrac{1}{2}(Q + iU), \tag{2.6a}$$

$$I_0 = E_{+1}E_{+1}{}^* = \tfrac{1}{2}(I + V), \tag{2.6b}$$

$$I_{-0} = E_{-1}E_{-1}{}^* = \tfrac{1}{2}(I - V), \tag{2.6c}$$

$$I_{-2} = E_{+1}E_{-1}{}^* = \tfrac{1}{2}(Q - iU), \tag{2.6d}$$

where the asterisk denotes the complex-conjugate value. The corresponding Stokes vectors (or intensity vectors) $\mathbf{I}^S$ and $\mathbf{I}^C$ are defined as (4×1) columns having the Stokes parameters as their components as follows:

$$\mathbf{I}^S = (I, Q, U, V)^T = \begin{bmatrix} I \\ Q \\ U \\ V \end{bmatrix}, \tag{2.7}$$

$$\mathbf{I}^C = (I_2, I_0, I_{-0}, I_{-2})^T = \begin{bmatrix} I_2 \\ I_0 \\ I_{-0} \\ I_{-2} \end{bmatrix}, \tag{2.8}$$

where T denotes matrix transposition.

C. Mueller Matrix of a Single Particle

Transformation of the Stokes parameters of the incident plane wave into those of the scattered spherical wave owing to light scattering by a single particle is given by (cf. Refs. 42 and 43)

$$\mathbf{I}_s^S(\hat{n}_s) = (1/r^2)\mathbf{Z}^S(\hat{n}_s;\hat{n}_i)\mathbf{I}_i^S(\hat{n}_i), \tag{2.9a}$$

$$\mathbf{I}_s^C(\hat{n}_s) = (1/r^2)\mathbf{Z}^C(\hat{n}_s;\hat{n}_i)\mathbf{I}_i^C(\hat{n}_i), \tag{2.9b}$$

where $\mathbf{Z}^S$ and $\mathbf{Z}^C$ are (4×4) Mueller matrices (or phase matrices). The elements of these matrices can easily be expressed in the elements of the amplitude scattering matrices. By using Eqs. (2.6) and (2.9b), we derive

$$\mathbf{Z}^C = \|Z_{pq}{}^C\| = \begin{bmatrix} C_{-1-1}C_{+1+1}{}^* & C_{-1+1}C_{+1+1}{}^* & C_{-1-1}C_{+1-1}{}^* & C_{-1+1}C_{+1-1}{}^* \\ C_{+1-1}C_{+1+1}{}^* & C_{+1+1}C_{+1+1}{}^* & C_{+1-1}C_{+1-1}{}^* & C_{+1+1}C_{+1-1}{}^* \\ C_{-1-1}C_{-1+1}{}^* & C_{-1+1}C_{-1+1}{}^* & C_{-1-1}C_{-1-1}{}^* & C_{-1+1}C_{-1-1}{}^* \\ C_{+1-1}C_{-1+1}{}^* & C_{+1+1}C_{-1+1}{}^* & C_{+1-1}C_{-1-1}{}^* & C_{+1+1}C_{-1-1}{}^* \end{bmatrix}, \quad p, q = 2, 0, -0, -2. \tag{2.10}$$

Also we have[4]

$$\mathbf{Z}^S = \mathbf{A}^{-1}\mathbf{Z}^C\mathbf{A}, \tag{2.11}$$

where

$$\mathbf{A} = \frac{1}{2}\begin{bmatrix} 0 & 1 & i & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & -i & 0 \end{bmatrix}, \quad \mathbf{A}^{-1} = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ -i & 0 & 0 & i \\ 0 & 1 & -1 & 0 \end{bmatrix}. \tag{2.12}$$

D. Mueller Matrices and Scattering Matrices of Ensembles of Randomly Oriented Particles

We now consider a small volume element containing N independently scattering particles. In this case the Stokes vectors of the waves scattered by the individual particles should be added to obtain the Stokes vector of the radiation scattered by the entire volume element.[44] Thus we have

$$\mathbf{Z}^{S,C}(\hat{n}_s;\hat{n}_i) = N\langle \mathbf{Z}^{S,C}(\hat{n}_s;\hat{n}_i)\rangle, \tag{2.13}$$

where the ensemble averaged Mueller matrices $\langle \mathbf{Z}^S\rangle$ and $\langle \mathbf{Z}^C\rangle$ are given by

$$\langle \mathbf{Z}^{S,C}(\hat{n}_s;\hat{n}_i)\rangle = \frac{1}{N}\sum_{n=1}^{N} \mathbf{Z}_n{}^{S,C}(\hat{n}_s;\hat{n}_i), \tag{2.14}$$

where n numbers the particles.

Now let the volume element be composed of identical, randomly oriented particles. In order to evaluate the ensemble averaged Mueller matrices, we find that it is convenient to introduce a special right-handed coordinate system A by attaching it firmly to the scattering particle. This coordinate system will be referred to as the natural reference frame (or body frame) of the scatterer. Orientation of each particle in the ensemble with respect to the laboratory reference frame B we define by the Eulerian angles of rotation α, β, and γ that transform the coordinate system B into the coordinate system A.[45] In that way, we can rewrite Eq. (2.14) as follows:

$$\langle \mathbf{Z}^{S,C}(\hat{n}_s;\hat{n}_i)\rangle = \frac{1}{8\pi^2}\int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \times \sin\beta \int_0^{2\pi} d\gamma\, \mathbf{Z}^{S,C}(\hat{n}_s;\hat{n}_i;\alpha\beta\gamma), \tag{2.15}$$

where $\mathbf{Z}^{S,C}(\hat{n}_s;\hat{n}_i;\alpha\beta\gamma)$ are the Mueller matrices of a particle with orientation $(\alpha\beta\gamma)$.

As follows from Eqs. (2.9a) and (2.9b), the Mueller matrices $\mathbf{Z}^S$ and $\mathbf{Z}^C$ relate the Stokes parameters of the incident and scattered radiation defined with respect to the corresponding meridional planes. Unlike the Mueller matrices, the scattering matrices $\mathbf{F}^S$ and $\mathbf{F}^C$ relate Stokes parameters defined with respect to the scattering plane (i.e., the plane through the vectors $\hat{n}_i$ and $\hat{n}_s$). Since for media consisting of randomly oriented particles the scattering matrices depend only on the scattering angle $\theta = \cos^{-1}(\hat{n}_s \cdot \hat{n}_i)$,[42,43] we define

$$\mathbf{F}^{S,C}(\theta) = \frac{4\pi}{C_{\text{sca}}}\langle \mathbf{Z}^{S,C}(\theta, 0; 0, 0)\rangle, \tag{2.16}$$

where the scattering cross section C_{sca} is defined as[42,43]

$$C_{\text{sca}} = \int_{4\pi} d\Omega \langle Z_{11}{}^S(\theta, 0; 0, 0)\rangle. \tag{2.17}$$

The factor $4\pi/C_{\text{sca}}$ in Eq. (2.16) is chosen such that the element (1, 1) of the scattering matrix $\mathbf{F}^S$ (the so-called phase function) satisfies the normalization condition

$$\frac{1}{4\pi}\int_{4\pi} d\Omega F_{11}{}^S(\theta) = 1. \tag{2.18}$$

E. Expansion of the Elements of the Scattering Matrices in Generalized Spherical Functions

In what follows, we shall assume that the scattering volume element consists of randomly oriented particles having a plane of symmetry and (or) particles and their mirror particles in equal numbers with random orientation. In this case the scattering matrix $\mathbf{F}^C$ has the form[1,4]

$$\mathbf{F}^C = \|F_{pq}{}^C\| = \frac{1}{2}\begin{bmatrix} a_2 + a_3 & b_1 + ib_2 & b_1 - ib_2 & a_2 - a_3 \\ b_1 + ib_2 & a_1 + a_4 & a_1 - a_4 & b_1 - ib_2 \\ b_1 - ib_2 & a_1 - a_4 & a_1 + a_4 & b_1 + ib_2 \\ a_2 - a_3 & b_1 - ib_2 & b_1 + ib_2 & a_2 + a_3 \end{bmatrix}, \quad p,q = 2, 0, -0, -2, \tag{2.19}$$

where a_1, a_2, a_3, a_4, b_1, and b_2 are some real functions of the scattering angle θ. As was mentioned above, a useful set of functions for making series expansions of the elements of this matrix is provided by so-called generalized spherical functions $P_{pq}{}^s(\cos\theta)$, which have been defined and exten-

sively studied by Gelfand *et al.*[46] (the principal properties of these functions are summarized in Appendix A). Following Refs. 1, 2, and 4, we write

$$F_{pq}{}^{C}(\theta) = \sum_{s=\max(|p|,|q|)}^{\infty} g_{pq}{}^{s} P_{pq}{}^{s}(\cos\theta), \qquad p, q = 2, 0, -0, -2, \quad (2.20)$$

where the expansion coefficients are given by [cf. Eq. (A9)]

$$g_{pq}{}^{s} = \frac{2s+1}{2} \int_{-1}^{+1} \mathrm{d}(\cos\theta) F_{pq}{}^{C}(\theta) P_{pq}{}^{s}(\cos\theta). \quad (2.21)$$

Note that for $P_{pq}{}^{s}(\cos\theta)$ no distinction is made between $p, q = 0$ or $p, q = -0$. By using Eqs. (2.19), (2.21), and (A8), we can easily derive the following symmetry relations[1]

$$g_{pq}{}^{s} = g_{qp}{}^{s} = g_{-p-q}{}^{s}, \quad (2.22)$$

$$g_{pp}{}^{s}, g_{p-p}{}^{s} = \text{real}, \qquad g_{20}{}^{s} = [g_{2-0}{}^{s}]^{*}. \quad (2.23)$$

Returning to the real-valued polarization parameters (I, Q, U, V), we have[42,43]

$$\mathbf{F}^{S} = \begin{bmatrix} a_1 & b_1 & 0 & 0 \\ b_1 & a_2 & 0 & 0 \\ 0 & 0 & a_3 & b_2 \\ 0 & 0 & -b_2 & a_4 \end{bmatrix}. \quad (2.24)$$

In this case the expansions [Eq. (2.20)] are replaced by the expansions[3,4,11,15,18]

$$a_1(\theta) = \sum_{s=0}^{\infty} a_1{}^{s} P_{00}{}^{s}(\cos\theta), \quad (2.25)$$

$$a_2(\theta) + a_3(\theta) = \sum_{s=2}^{\infty} (a_2{}^{s} + a_3{}^{s}) P_{22}{}^{s}(\cos\theta), \quad (2.26)$$

$$a_2(\theta) - a_3(\theta) = \sum_{s=2}^{\infty} (a_2{}^{s} - a_3{}^{s}) P_{2-2}{}^{s}(\cos\theta), \quad (2.27)$$

$$a_4(\theta) = \sum_{s=0}^{\infty} a_4{}^{s} P_{00}{}^{s}(\cos\theta), \quad (2.28)$$

$$b_1(\theta) = \sum_{s=2}^{\infty} b_1{}^{s} P_{02}{}^{s}(\cos\theta), \quad (2.29)$$

$$b_2(\theta) = \sum_{s=2}^{\infty} b_2{}^{s} P_{02}{}^{s}(\cos\theta), \quad (2.30)$$

where

$$a_1{}^{s} = g_{00}{}^{s} + g_{0-0}{}^{s}, \quad (2.31)$$

$$a_2{}^{s} = g_{22}{}^{s} + g_{2-2}{}^{s}, \quad (2.32)$$

$$a_3{}^{s} = g_{22}{}^{s} - g_{2-2}{}^{s}, \quad (2.33)$$

$$a_4{}^{s} = g_{00}{}^{s} - g_{0-0}{}^{s}, \quad (2.34)$$

$$b_1{}^{s} = 2\,\mathrm{Re}\, g_{02}{}^{s}, \quad (2.35)$$

$$b_2{}^{s} = 2\,\mathrm{Im}\, g_{02}{}^{s}. \quad (2.36)$$

Note that Eq. (2.25) is the well-known expansion of the phase function in Legendre polynomials[47–49] [cf. Eq. (A4)]. From the normalization condition [Eq. (2.18)], we have the identity

$$a_1{}^{0} = 1. \quad (2.37)$$

3. *T*-MATRIX ANSATZ

A. Amplitude Scattering Matrix

For calculating the elements of the amplitude scattering matrix $\mathbf{S}(\hat{n}_s; \hat{n}_i)$ for a single nonspherical particle with a fixed orientation with respect to the laboratory reference frame, we use the T-matrix approach.[29] Thus we expand the incident and scattered fields in vector spherical waves $\mathbf{M}_{mn}$ and $\mathbf{N}_{mn}$ as follows[50]:

$$\mathbf{E}^{i}(\mathbf{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} [a_{mn}\,\mathrm{Rg}\,\mathbf{M}_{mn}(k\mathbf{r}) + b_{mn}\,\mathrm{Rg}\,\mathbf{N}_{mn}(k\mathbf{r})], \quad (3.1)$$

$$\mathbf{E}^{s}(\mathbf{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} [p_{mn}\mathbf{M}_{mn}(k\mathbf{r}) + q_{mn}\mathbf{N}_{mn}(k\mathbf{r})], \qquad r > r_0, \quad (3.2)$$

where

$$\mathbf{M}_{mn}(k\mathbf{r}) = (-1)^{m} d_n h_n^{(1)}(kr) \mathbf{C}_{mn}(\theta) \exp(im\varphi), \quad (3.3)$$

$$\mathbf{N}_{mn}(k\mathbf{r}) = (-1)^{m} d_n \left\{ \frac{n(n+1)}{kr} h_n^{(1)}(kr) \mathbf{P}_{mn}(\theta) + \frac{1}{kr} [kr h_n^{(1)}(kr)]' \mathbf{B}_{mn}(\theta) \right\} \exp(im\varphi), \quad (3.4)$$

$$\mathbf{B}_{mn}(\theta) = \hat{\theta} \frac{\mathrm{d}}{\mathrm{d}\theta} d_{0m}{}^{n}(\theta) + \hat{\varphi} \frac{im}{\sin\theta} d_{0m}{}^{n}(\theta), \quad (3.5)$$

$$\mathbf{C}_{mn}(\theta) = \hat{\theta} \frac{im}{\sin\theta} d_{0m}{}^{n}(\theta) - \hat{\varphi} \frac{\mathrm{d}}{\mathrm{d}\theta} d_{0m}{}^{n}(\theta), \quad (3.6)$$

$$\mathbf{P}_{mn}(\theta) = \hat{r} d_{0m}{}^{n}(\theta), \quad (3.7)$$

$$d_n = \left[\frac{2n+1}{4\pi n(n+1)} \right]^{1/2}, \quad (3.8)$$

and r_0 is the radius of a circumscribing sphere of the scattering particle. Wigner functions $d_{mm'}{}^{n}(\theta)$ are expressed in the generalized spherical functions as follows:

$$d_{mm'}{}^{n}(\theta) = i^{m'-m} P_{mm'}{}^{n}(\cos\theta). \quad (3.9)$$

The expressions for the functions $\mathrm{Rg}\,\mathbf{M}_{mn}$ and $\mathrm{Rg}\,\mathbf{N}_{mn}$ can be obtained from Eqs. (3.3) and (3.4) by replacing spherical Hankel functions $h_n^{(1)}$ by spherical Bessel functions j_n.

From the linearity of Maxwell's equations and boundary conditions, the relation between the scattered field coefficients and exciting field coefficients is linear and is given by a transition matrix (or T matrix) $\mathbf{T}$ as follows:

$$p_{mn} = \sum_{n'=1}^{\infty} \sum_{m'=-n'}^{n'} (T_{mnm'n'}{}^{11} a_{m'n'} + T_{mnm'n'}{}^{12} b_{m'n'}), \quad (3.10)$$

$$q_{mn} = \sum_{n'=1}^{\infty} \sum_{m'=-n'}^{n'} (T_{mnm'n'}{}^{21} a_{m'n'} + T_{mnm'n'}{}^{22} b_{m'n'}). \quad (3.11)$$

The elements of the T matrix do not depend on the directions of propagation and the states of polarization of the incident and scattered fields. They depend only on the size,

morphology, and composition of the scattering particle as well as on its orientation with respect to the laboratory reference frame.

For a plane incident wave

$$\mathbf{E}^i(\mathbf{r}) = \mathbf{E}_i \exp(ik\hat{n}_i\mathbf{r}), \tag{3.12}$$

the expansion coefficients a_{mn} and b_{mn} are[45,50]

$$a_{mn} = 4\pi(-1)^m i^n d_n \mathbf{C}_{mn}^*(\theta_i)\mathbf{E}_i \exp(-im\varphi_i), \tag{3.13}$$

$$b_{mn} = 4\pi(-1)^m i^{n-1} d_n \mathbf{B}_{mn}^*(\theta_i)\mathbf{E}_i \exp(-im\varphi_i). \tag{3.14}$$

By making use of the large argument approximation for spherical Henkel functions,

$$h_n^{(1)}(kr) \simeq \frac{(-i)^{n+1}\exp(ikr)}{kr}, \qquad kr \gg n^2, \tag{3.15}$$

and taking into account Eqs. (2.2), (3.2)–(3.4), and (3.10)–(3.14), we obtain an expression of the elements of the amplitude scattering matrix $\mathbf{S}$ in terms of the T-matrix elements. In dyadic notation we have[29,50]

$$\mathbf{S}(\hat{n}_s; \hat{n}_i) = \frac{4\pi}{k} \sum_{nmn'm'} i^{n'-n-1}(-1)^{m+m'} \mathrm{d}_n \mathrm{d}_{n'} \exp[i(m\varphi_s - m'\varphi_i)]$$
$$\times \{[T_{mnm'n'}{}^{11}\mathbf{C}_{mn}(\theta_s) + T_{mnm'n'}{}^{21} i\mathbf{B}_{mn}(\theta_s)]\mathbf{C}_{m'n'}{}^*(\theta_i)$$
$$+ [T_{mnm'n'}{}^{12}\mathbf{C}_{mn}(\theta_s) + T_{mnm'n'}{}^{22} i\mathbf{B}_{mn}(\theta_s)]\mathbf{B}_{m'n'}{}^*(\theta_i)/i\}. \tag{3.16}$$

B. Rotations of the Coordinate System

Let ${}^1\mathbf{T}$ and ${}^2\mathbf{T}$ be the T matrices of a particle calculated with respect to arbitrary coordinate systems 1 and 2, respectively, and let α, β, and γ be the Eulerian angles of rotation that transform the coordinate system 2 into the coordinate system 1. By using the expansion[45,50]

$$\mathbf{M}_{mn}(kr, \theta_1, \varphi_1) = \sum_{m'=-n}^{n} D_{m'm}{}^n(\alpha\beta\gamma)\mathbf{M}_{m'n}(kr, \theta_2, \varphi_2), \tag{3.17}$$

where

$$D_{m'm}{}^n(\alpha\beta\gamma) = \exp(-im'\alpha)d_{m'm}{}^n(\beta)\exp(-im\gamma) \tag{3.18}$$

are Wigner D functions, and similar expressions for the functions $\mathbf{N}_{mn}$, Rg $\mathbf{M}_{mn}$, and Rg $\mathbf{N}_{mn}$ and taking into account Eqs. (3.1), (3.2), (3.10), and (3.11), we derive[50,51]

$${}^2T_{mnm'n'}{}^{ij} = \sum_{m_1=-n}^{n} \sum_{m_2=-n'}^{n'} D_{m_2m'}{}^{-1\,n'}(\alpha\beta\gamma)$$
$$\times {}^1T_{m_1nm_2n'}{}^{ij} D_{mm_1}{}^n(\alpha\beta\gamma), \qquad i, j = 1, 2, \tag{3.19}$$

where

$$D_{m_2m'}{}^{-1\,n'}(\alpha\beta\gamma) = [D_{m'm_2}{}^{n'}(\alpha\beta\gamma)]^* = D_{m_2m'}{}^{n'}(-\gamma - \beta - \alpha). \tag{3.20}$$

It is worthwhile to note that the sums of the diagonal elements of the matrices $\mathbf{T}^{ij}(i, j = 1, 2)$ are invariant with respect to the rotations of the coordinate system. By using Eqs. (3.18) and (3.19) and taking into account that[45]

$$\sum_{m=-n}^{n} d_{mm_1}{}^n(\beta)d_{mm_2}{}^n(\beta) = \delta_{m_1m_2}, \tag{3.21}$$

where $\delta_{m_1m_2}$ is the Kronecker delta, we easily derive

$$\sum_{n=1}^{\infty} \sum_{m=-n}^{n} {}^2T_{mnmn}{}^{ij} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} {}^1T_{mnmn}{}^{ij}, \qquad i, j = 1, 2. \tag{3.22}$$

This property is in agreement with the formula[52]

$$C_{\mathrm{ext}} = -\frac{2\pi}{k^2} \mathrm{Re} \sum_{n=1}^{\infty} \sum_{m=-n}^{n} (T_{mnmn}{}^{11} + T_{mnmn}{}^{22}), \tag{3.23}$$

where C_{ext} is the extinction cross section averaged over an ensemble of randomly oriented identical particles and $\mathbf{T}$ is the T matrix of a single particle calculated with respect to an arbitrarily chosen reference frame.

C. Axially Symmetric Scatterers

In principle, the T-matrix approach can be applied to an isotropic particle with any (even rather complicated) shape and internal structure (see, e.g., Ref. 53, in which theory and numerical results for general ellipsoids are reported). Nevertheless, both mathematics and computer calculations become much simpler if the scattering particle (homogeneous or composite) is axially symmetric.[38,54,55] Therefore, in what follows, we shall assume that the shape and the refractive index m_r of the scattering particle in the natural reference frame A can be specified by equations

$$r(\theta, \varphi) = r(\theta), \tag{3.24}$$

$$m_r(r, \theta, \varphi) = m_r(r, \theta). \tag{3.25}$$

In other words, the z axis of the natural reference frame is chosen to be the axis of particle symmetry.

Let $\mathbf{T}(A)$ be the T matrix of an axially symmetric scatterer calculated with respect to its natural reference frame and let the natural reference frame be coincident with the laboratory reference frame. Then the amplitude scattering matrix $\mathbf{S}$ should possess the properties[42,43]

$$\mathbf{S}(\hat{n}_s; \hat{n}_i) = \mathbf{S}(\theta_s, \theta_i, \varphi_s - \varphi_i), \tag{3.26}$$

$$\mathbf{S}(\theta_s, \theta_i, \varphi_s - \varphi_i) = \mathbf{Q}\mathbf{S}(\theta_s, \theta_i, \varphi_i - \varphi_s)\mathbf{Q}, \tag{3.27}$$

where $\mathbf{Q} = \mathrm{diag}(1, -1)$. As a result, by using Eq. (3.16) and the symmetry relation [cf. Eqs. (3.9) and (A8)]

$$d_{mm'}{}^n(\theta) = (-1)^{m+m'} d_{-m-m'}{}^n(\theta), \tag{3.28}$$

we have

$$T_{mnm'n'}{}^{ij}(A) = \delta_{mm'} T_{mnn'}{}^{ij}(A), \tag{3.29}$$

$$T_{mnn'}{}^{ij}(A) = (-1)^{i+j} T_{-mnn'}{}^{ij}(A). \tag{3.30}$$

4. EXPANSION OF THE ELEMENTS OF THE SCATTERING MATRICES OF ENSEMBLES OF RANDOMLY ORIENTED AXIALLY SYMMETRIC PARTICLES IN GENERALIZED SPHERICAL FUNCTIONS

Consider an axially symmetric particle having orientation $(\alpha\beta\gamma)$ with respect to the laboratory reference frame B. We denote by $\mathbf{T}(\alpha\beta\gamma)$ the T matrix of this particle calculated with respect to the laboratory frame and by $\mathbf{C}(\hat{n}_s; \hat{n}_i; \alpha\beta\gamma)$ and $\mathbf{S}(\hat{n}_s; \hat{n}_i; \alpha\beta\gamma)$ the corresponding amplitude scattering

matrices. By using Eqs. (2.4), (3.5), (3.6), and (3.16) and taking into account the formulas[45]

$$\frac{m}{\sin\theta} d_{0m}{}^{n}(\theta)|_{\theta=0} = \delta_{m\pm1}\tfrac{1}{2}[n(n+1)]^{1/2}, \tag{4.1}$$

$$\frac{\mathrm{d}}{\mathrm{d}\theta} d_{0m}{}^{n}(\theta)|_{\theta=0} = m\delta_{m\pm1}\tfrac{1}{2}[n(n+1)]^{1/2}, \tag{4.2}$$

$$\frac{m}{\sin\theta} d_{0m}{}^{n}(\theta) = \tfrac{1}{2}[n(n+1)]^{1/2}[d_{1m}{}^{n}(\theta) + d_{-1m}{}^{n}(\theta)], \tag{4.3}$$

$$\frac{\mathrm{d}}{\mathrm{d}\theta} d_{0m}{}^{n}(\theta) = \tfrac{1}{2}[n(n+1)]^{1/2}[d_{1m}{}^{n}(\theta) - d_{-1m}{}^{n}(\theta)], \tag{4.4}$$

we find that

$$\begin{aligned} C_{+1+1}(\theta, 0; 0, 0; \alpha\beta\gamma) = \sum_{n=1}^{\infty}\sum_{n'=1}^{\infty}\sum_{m=-n}^{n} t_{mnn'} d_{-1m}{}^{n}(\theta) \\ \times [T_{mn-1n'}{}^{11}(\alpha\beta\gamma) - T_{mn-1n'}{}^{12}(\alpha\beta\gamma) \\ - T_{mn-1n'}{}^{21}(\alpha\beta\gamma) + T_{mn-1n'}{}^{22}(\alpha\beta\gamma)], \end{aligned} \tag{4.5}$$

$$\begin{aligned} C_{+1-1} = \sum_{nn'm} t_{mnn'} d_{-1m}{}^{n}[T_{mn1n'}{}^{11} + T_{mn1n'}{}^{12} \\ - T_{mn1n'}{}^{21} - T_{mn1n'}{}^{22}], \end{aligned} \tag{4.6}$$

$$\begin{aligned} C_{-1+1} = \sum_{nn'm} t_{mnn'} d_{1m}{}^{n}[T_{mn-1n'}{}^{11} - T_{mn-1n'}{}^{12} \\ + T_{mn-1n'}{}^{21} - T_{mn-1n'}{}^{22}], \end{aligned} \tag{4.7}$$

$$\begin{aligned} C_{-1-1} = \sum_{nn'm} t_{mnn'} d_{1m}{}^{n}[T_{mn1n'}{}^{11} + T_{mn1n'}{}^{12} \\ + T_{mn1n'}{}^{21} + T_{mn1n'}{}^{22}], \end{aligned} \tag{4.8}$$

where

$$t_{mnn'} = \frac{1}{2k} i^{n'-n-1}(-1)^{m+1}[(2n+1)(2n'+1)]^{1/2}. \tag{4.9}$$

Note that all the arguments in Eqs. (4.6)–(4.8) have been omitted for brevity. Then, we use Eqs. (3.19), (3.28)–(3.30), and (4.5)–(4.9) together with the formulas[45]

$$\begin{aligned} d_{mm'}{}^{n}(\theta) d_{m_1m_1'}{}^{n'}(\theta) = \sum_{n_1=|n-n'|}^{n+n'} C_{nm\,n'm_1}{}^{n_1m+m_1} C_{nm'\,n'm_1'}{}^{n_1m'+m_1'} \\ \times d_{m+m_1m'+m_1'}{}^{n_1}(\theta), \end{aligned} \tag{4.10}$$

$$C_{n_1m_1\,n_2m_2}{}^{nm} = (-1)^{n_1+m_1}\left(\frac{2n+1}{2n_2+1}\right)^{1/2} C_{n_1m_1\,n-m}{}^{n_2-m_2}, \tag{4.11}$$

$$C_{n_1m_1\,n_2m_2}{}^{nm} = (-1)^{n+n_1+n_2} C_{n_1-m_1\,n_2-m_2}{}^{n-m} \tag{4.12}$$

to derive

$$\begin{aligned} C_{+1+1}(\theta, 0; 0, 0; \alpha\beta\gamma) = \sum_{n=1}^{\infty}\sum_{m=-n}^{n}\sum_{n_1=|m-1|}^{\infty} f_{nn_1} d_{-1-m}{}^{n}(\theta) \\ \times d_{1-m0}{}^{n_1}(\beta)\exp[-i\alpha(1-m)] B_{mnn_1}{}^{1}, \end{aligned} \tag{4.13}$$

$$C_{+1-1} = \sum_{nmn_1} f_{nn_1} d_{-1m}{}^{n} d_{m-10}{}^{n_1} \exp[-i\alpha(m-1)] B_{mnn_1}{}^{2}, \tag{4.14}$$

$$C_{-1+1} = \sum_{nmn_1} f_{nn_1} d_{-1m}{}^{n} d_{m-0}{}^{n_1} \exp[-i\alpha(1-m)] B_{mnn_1}{}^{2}, \tag{4.15}$$

$$C_{-1-1} = \sum_{nmn_1} f_{nn_1} d_{1-m}{}^{n} d_{1-m0}{}^{n_1} \exp[-i\alpha(m-1)] B_{mnn_1}{}^{1}, \tag{4.16}$$

where $f_{nn_1} = (2n+1)^{1/2}(2n_1+1)/(2ik)$,

$$B_{mnn_1}{}^{j} = \sum_{n'=\max(1,|n-n_1|)}^{n+n_1} C_{nm\,n_1 1-m}{}^{n'1} A_{nn'n_1}{}^{j}, \qquad j = 1, 2, \tag{4.17}$$

$$A_{nn'n_1}{}^{j} = \frac{i^{n'-n}}{(2n'+1)^{1/2}} \sum_{m_1=-M_1}^{M_1} C_{nm_1\,n_1 0}{}^{n'm_1} T_{m_1nn'}{}^{j}, \qquad M_1 = \min(n, n'), \tag{4.18}$$

$$T_{mnn'}{}^{1} = T_{mnn'}{}^{11}(A) + T_{mnn'}{}^{12}(A) + T_{mnn'}{}^{21}(A) + T_{mnn'}{}^{22}(A), \tag{4.19}$$

$$T_{mnn'}{}^{2} = T_{mnn'}{}^{11}(A) + T_{mnn'}{}^{12}(A) - T_{mnn'}{}^{21}(A) - T_{mnn'}{}^{22}(A). \tag{4.20}$$

Here, $T_{mnn'}{}^{ij}(A)$ are elements of the T matrix of the axially symmetric scatterer calculated with respect to its natural reference frame A (cf. Subsection 3.C) and $C_{n_1m_1\,n_2m_2}{}^{mn}$ are Clebsch–Gordan coefficients related to Wigner $3j$ symbols by[45]

$$C_{n_1m_1\,n_2m_2}{}^{nm} = (-1)^{n_1+n_2+m}(2n+1)^{1/2}\begin{bmatrix} n_1 & n_2 & n \\ m_1 & m_2 & -m \end{bmatrix}. \tag{4.21}$$

Finally, by using Eqs. (2.10), (2.15), (2.16), (2.20), (3.9), (3.28), and (4.10)–(4.16) together with the orthogonality relation [cf. Eqs. (3.9) and (A9)]

$$\int_0^{\pi} \mathrm{d}\beta \sin\beta d_{mm_1}{}^{n}(\beta) d_{mm_1}{}^{n'}(\beta) = \delta_{nn'}\frac{2}{2n+1}, \tag{4.22}$$

we obtain the following formulas that can be used in practical computer calculations:

$$g_{00}{}^{s} = \sum_{n=1}^{\infty}\sum_{\hat{n}=\max(1,|n-s|)}^{n+s} h_{sn\hat{n}} C_{n1\,s0} \sum_{m=-M}^{M} C_{nm\,s0}{}^{\hat{n}m} D_{mn\hat{n}}{}^{00}, \tag{4.23}$$

$$g_{0-0}{}^{s} = \sum_{n\hat{n}} h_{sn\hat{n}}(-1)^{n+\hat{n}+s} C_{n1\,s0}{}^{\hat{n}1} \sum_{m=-M}^{M} C_{nm\,s0}{}^{\hat{n}m} D_{mn\hat{n}}{}^{0-0}, \tag{4.24}$$

$$g_{22}{}^{s} = \sum_{n\hat{n}} h_{sn\hat{n}} C_{n-1\,s2}{}^{\hat{n}1} \sum_{m=m_{\min}}^{m_{\max}} C_{n-m\,s2}{}^{\hat{n}2-m} D_{mn\hat{n}}{}^{22}, \tag{4.25}$$

$$g_{2-2}{}^{s} = \sum_{n\hat{n}} h_{sn\hat{n}}(-1)^{n+\hat{n}+s} C_{n-1\,s2}{}^{\hat{n}1} \sum_{m=m_{\min}}^{m_{\max}} C_{n-m\,s2}{}^{\hat{n}2-m} D_{mn\hat{n}}{}^{2-2}, \tag{4.26}$$

$$g_{02}{}^{s} = -\sum_{n\hat{n}} h_{sn\hat{n}} C_{n1\,s0}{}^{\hat{n}1} \sum_{m=m_{\min}}^{m_{\max}} C_{n-m\,s2}{}^{\hat{n}2-m} D_{mn\hat{n}}{}^{02}, \tag{4.27}$$

where

$$h_{sn\hat{n}} = \frac{(2s+1)\pi}{k^2 C_{\text{sca}}} \left(\frac{2n+1}{2\hat{n}+1}\right)^{1/2}, \tag{4.28}$$

$$D_{mn\hat{n}}{}^{00} = \sum_{n_1=|m-1|}^{\infty} (2n_1+1) B_{mnn_1}{}^{1} (B_{m\hat{n}n_1}{}^{1})^*, \tag{4.29}$$

$$D_{mn\hat{n}}{}^{0-0} = \sum_{n_1} (2n_1+1) B_{mnn_1}{}^{2} (B_{m\hat{n}n_1}{}^{2})^*, \tag{4.30}$$

$$D_{mn\hat{n}}{}^{22} = \sum_{n_1} (2n_1+1) B_{mnn_1}{}^{1} (B_{2-m\hat{n}n_1}{}^{1})^*, \tag{4.31}$$

$$D_{mn\hat{n}}{}^{2-2} = \sum_{n_1} (2n_1+1) B_{mnn_1}{}^{2} (B_{2-m\hat{n}n_1}{}^{2})^*, \tag{4.32}$$

$$D_{mn\hat{n}}{}^{02} = \sum_{n_1} (2n_1+1) B_{mnn_1}{}^{2} (B_{2-m\hat{n}n_1}{}^{1})^*. \tag{4.33}$$

$M = \min(n, \hat{n})$, $m_{\min} = \max(-n, -\hat{n}+2)$, and $m_{\max} = \min(n, \hat{n}+2)$. An expression for C_{sca} can be derived by using Eqs. (2.31), (2.37), (3.30), (4.11), (4.17)–(4.20), (4.23), (4.24), and (4.28)–(4.30) together with the formulas[45]

$$C_{n_1 m_1\,00}{}^{nm} = \delta_{nn_1}\delta_{mm_1}, \tag{4.34}$$

$$\sum_{m_1 m_2} C_{n_1 m_1\,n_2 m_2}{}^{nm} C_{n_1 m_1\,n_2 m_2}{}^{n'm'} = \delta_{nn'}\delta_{mm'}, \tag{4.35}$$

$$\sum_{nm} C_{n_1 m_1\,n_2 m_2}{}^{nm} C_{n_1 m_1'\,n_2 m_2'}{}^{nm} = \delta_{m_1 m_1'}\delta_{m_2 m_2'}. \tag{4.36}$$

After some manipulations, we get[56]

$$C_{\text{sca}} = \frac{2\pi}{k^2} \sum_{n=1}^{\infty} \sum_{n'=1}^{\infty} \sum_{m=0}^{\min(n,n')} \sum_{i,j=1,2} (2-\delta_{m0}) |T_{mnn'}{}^{ij}(A)|^2. \tag{4.37}$$

It is worthwhile to note that, for a spherical particle with spherically symmetric internal structure,

$$T_{mnn'}{}^{11}(A) = -\delta_{nn'} b_n, \tag{4.38}$$

$$T_{mnn'}{}^{22}(A) = -\delta_{nn'} a_n, \tag{4.39}$$

$$T_{mnn'}{}^{12}(A) = T_{mnn'}{}^{21}(A) = 0, \tag{4.40}$$

where a_n and b_n are the Mie coefficients, if the particle is homogeneous, and their analogs, if the particle is radially inhomogeneous. In this case our expressions (4.23)–(4.27) can easily be reduced to those derived earlier in Refs. 10, 24, 26, and 27.

5. PRACTICAL CONSIDERATIONS AND NUMERICAL RESULTS

A. Computational Aspects

There are eight major numerical steps involved in the computation of the expansion coefficients $a_1{}^s, \ldots, b_2{}^s$ and the elements of the scattering matrix $\mathbf{F}^S(\theta)$:

(1) Computation of the T matrix of an axially symmetric (homogeneous or composite) scatterer with respect to its natural reference frame with the z axis along the axis of symmetry [i.e., the matrix $\mathbf{T}(A)$].

(2) Computation of the quantities $T_{mnn'}{}^{j}$, $j = 1, 2$ [Eqs. (4.19) and (4.20)].

(3) Computation of the quantities $A_{nn'n_1}{}^{j}$ [Eq. (4.18)].

(4) Computation of the quantities $B_{mnn_1}{}^{j}$ [Eq. (4.17)].

(5) Computation of the quantities $D_{mn\hat{n}}{}^{pq}$ [Eqs. (4.29)–(4.33)].

(6) Computation of the expansion coefficients $g_{pq}{}^{s}$ [Eqs. (4.23)–(4.27)].

(7) Computation of the expansion coefficients $a_1{}^s, \ldots, b_2{}^s$ [Eqs. (2.31)–(2.36)].

(8) Computation of the elements of the scattering matrix $\mathbf{F}^S(\theta)$ [Eqs. (2.25)–(2.30)].

Note that step (1) is the first and the necessary step in any computations based on the T-matrix approach.

Formulas for computing the matrix $\mathbf{T}(A)$ for homogeneous axially symmetric particles are given, e.g., by Tsang *et al.*[50] The corresponding computational aspects are extensively discussed by Wiscombe and Mugnai[38] [note, however, that these authors used another set of vector spherical wave functions in the expansions (3.1) and (3.2)]. Computation of the T matrix for composite particles is considered in Refs. 33, 39–41, and 57.

Formulas for computing the Clebsch–Gordan coefficients, appearing in Eqs. (4.17), (4.18), and (4.23)–(4.27), are given in Appendix B. Formulas for computing the generalized spherical functions, appearing in Eqs. (2.25)–(2.30), are given in Appendix A.

B. Illustrative Numerical Results and Timing Tests

In this subsection we present results of numerical computations for randomly oriented, identical homogeneous dielectric spheroids and Chebyshev particles. The surface of a spheroid in the natural coordinate system A is governed by the equation

$$r(\theta, \varphi) = a(\sin^2\theta + d^2\cos^2\theta)^{-1/2}, \qquad d = a/b, \tag{5.1}$$

where b is the rotational semiaxis and a is the horizontal semiaxis of the spheroid. The surface of a Chebyshev particle is governed by the equation[34]

$$r(\theta, \varphi) = r_0(1 + E\cos n\theta). \tag{5.2}$$

Computations in Tables 1–5 are reported for two models:

Model 1[58]: Prolate spheroids with a refractive index $m_r = 1.5 + 0.1i$, $a/b = 1/2$, and a size parameter $kb = 5.5$.

Model 2[38]: Chebyshev particles with $m_r = 1.5 + 0.02i$, $n = 3$, $E = 0.1$, and $kr_{\text{ev}} = 3$, where r_{ev} is the radius of the equal-volume sphere.

Table 1. Expansion Coefficients for Model 1

s	a_1^s	a_2^s	a_3^s	a_4^s	b_1^s	b_2^s
0	1.000000	0.0	0.0	0.943446	0.0	0.0
1	2.449550	0.0	0.0	2.421722	0.0	0.0
2	3.123660	4.180223	4.109855	3.106991	0.012793	−0.065569
3	3.142994	3.913184	3.858398	3.154976	−0.033159	−0.194309
4	2.648942	3.318048	3.245528	2.646169	0.000931	−0.333894
5	1.852605	2.358863	2.311293	1.858816	0.131249	−0.352652
6	1.121077	1.422789	1.378063	1.118224	0.178267	−0.223151
7	0.580167	0.737566	0.707019	0.574649	0.131081	−0.114392
8	0.267070	0.338191	0.320543	0.263145	0.077582	−0.056100
9	0.104690	0.133785	0.123587	0.101423	0.041087	−0.024463
10	0.035834	0.045959	0.040628	0.033490	0.017860	−0.008191
11	0.010102	0.012998	0.010819	0.008953	0.006184	−0.002302
12	0.002459	0.003153	0.002441	0.002035	0.001730	−0.000496
13	0.000502	0.000641	0.000457	0.000384	0.000394	−0.000092
14	0.000089	0.000112	0.000074	0.000062	0.000075	−0.000014
15	0.000013	0.000017	0.000010	0.000009	0.000012	−0.000002
16	0.000002	0.000002	0.000001	0.000001	0.000002	−0.000000
17	0.000000	0.000000	0.000000	0.000000	0.000000	−0.000000

Table 2. Expansion Coefficients for Model 2

s	a_1^s	a_2^s	a_3^s	a_4^s	b_1^s	b_2^s
0	1.000000	0.0	0.0	0.938406	0.0	0.0
1	2.239020	0.0	0.0	2.243909	0.0	0.0
2	2.626152	3.971995	3.863824	2.602063	−0.029173	−0.128099
3	2.263763	3.057403	3.043574	2.362567	−0.083886	−0.307404
4	1.443307	2.254530	2.111606	1.428102	−0.024388	−0.503761
5	0.642610	0.946340	0.907134	0.667351	0.253410	−0.349050
6	0.246465	0.386070	0.329076	0.230343	0.145396	−0.071618
7	0.058742	0.091230	0.070889	0.050131	0.046878	−0.012777
8	0.010306	0.015634	0.010531	0.007648	0.009644	−0.001458
9	0.001385	0.002043	0.001170	0.000874	0.001409	−0.000118
10	0.000148	0.000213	0.000103	0.000079	0.000158	−0.000007
11	0.000013	0.000018	0.000007	0.000006	0.000014	−0.000000
12	0.000001	0.000001	0.000000	0.000000	0.000001	−0.000000
13	0.000000	0.000000	0.000000	0.000000	0.000000	−0.000000

In Tables 1 and 2 computed values of the expansion coefficients $a_1^s, \ldots, b_2^s$ are given. In Tables 3 and 4 these coefficients are used to compute the elements of the corresponding scattering matrices for a number of scattering angles. The computed values of the efficiency factors for extinction, Q_{ext}, for scattering, Q_{sca}, and for absorption, Q_{abs}, as well as the single scattering albedo w and the asymmetry parameter of the phase function $\langle \cos\theta \rangle$, are presented in Table 5 and are given by

$$Q_{\text{ext}} = C_{\text{ext}}/S, \tag{5.3}$$

$$Q_{\text{sca}} = C_{\text{sca}}/S, \tag{5.4}$$

$$Q_{\text{abs}} = Q_{\text{ext}} - Q_{\text{sca}}, \tag{5.5}$$

$$w = C_{\text{sca}}/C_{\text{ext}}, \tag{5.6}$$

$$\langle \cos\theta \rangle = \tfrac{1}{2}\int_{-1}^{+1} \mathrm{d}(\cos\theta) a_1(\theta)\cos\theta = a_1^1/3, \tag{5.7}$$

where $S = \pi r_{\text{ev}}^2$ is the geometrical cross section of the equal-volume sphere. Extinction cross sections C_{ext} and scattering cross sections C_{sca} were computed by using Eqs. (3.23) and (4.37).

Table 6 presents the results of timing tests for the two models, illustrating the speed of this method. In this table t_T is the time for computing the T matrix of an axially symmetric scatterer with respect to its natural reference frame [step (1)], t_a is the time for computing the expansion coefficients $a_1^s, \ldots, b_2^s$ [steps (2)–(7)], and t_F is the time for computing the elements of the scattering matrix $\mathbf{F}^S$ for one value of the scattering angle. All the times are in seconds on an ES 1061 computer. Also, in Table 6 the computational parameters $n_{\max}$ and N_G are the highest n value in the expansions (3.1) and (3.2) and the number of Gaussian quadrature points used in computing surface integrals, respectively (see, e.g., Secs. V and VI of Ref. 38).

It is seen from Table 6 that the computer times for calculating the expansion coefficients are roughly equal to those

Table 3. Elements of the Scattering Matrix for Model 1

θ	a_1	a_2	a_3	a_4	b_1	b_2
0°	16.3398	16.2871	16.2871	16.2345	0.0	0.0
30°	4.9774	4.9449	4.9043	4.8938	−0.2142	0.5491
60°	0.2987	0.2835	0.2156	0.2257	0.0976	0.0596
90°	0.1459	0.1220	0.0755	0.0970	−0.0471	−0.0340
120°	0.0621	0.0356	0.0027	0.0272	−0.0095	0.0103
150°	0.0326	0.0244	−0.0197	−0.0132	0.0024	−0.0058
180°	0.0585	0.0329	−0.0329	−0.0074	0.0	0.0

Table 4. Elements of the Scattering Matrix for Model 2

θ	a_1	a_2	a_3	a_4	b_1	b_2
0°	10.5319	10.5317	10.5317	10.5315	0.0	0.0
30°	5.0859	5.0835	5.0522	5.0502	−0.1765	0.5337
60°	0.5330	0.5295	0.4353	0.4335	0.1626	0.2424
90°	0.1539	0.1520	0.1029	0.1030	−0.0357	−0.0982
120°	0.1338	0.1325	0.1150	0.1150	−0.0268	0.0501
150°	0.0731	0.0722	−0.0310	−0.0314	0.0600	−0.0011
180°	0.1208	0.1195	−0.1195	−0.1182	0.0	0.0

Table 5. Computed Values of Extinction Efficiency Factor Q_{ext}, Scattering Efficiency Factor Q_{sca}, Absorption Efficiency Factor Q_{abs}, Albedo for Single Scattering w, and Asymmetry Parameter of the Phase Function $\langle \cos\theta \rangle$

Model	Q_{ext}	Q_{sca}	Q_{abs}	w	$\langle \cos\theta \rangle$
1	3.28535	2.29028	0.99507	0.69712	0.81652
2	3.31029	3.05078	0.25951	0.92161	0.74634

Table 6. Computer Times for Calculating the $T(A)$ Matrix, t_T, the Expansion Coefficients, t_a, and the Elements of the Scattering Matrix for One Value of the Scattering Angle t_F[a]

Model	t_T	t_a	t_F	Computational Parameters $n_{\max}$	Computational Parameters N_G
1	35.38	38.81	0.0081	16	50
2	68.96	44.77	0.0071	17	50

[a] Times are in seconds on an ES 1061 computer.

for calculating the matrices $\mathbf{T}(A)$ for the homogeneous axially symmetric scatterers. As was noted above, the time t_T is the minimum computer time for any computations based on the T-matrix approach. Thus, by using the method proposed to compute the expansion coefficients for randomly oriented scatterers, we only double this minimum time. Also, $t_F \ll t_T$ and $t_F \ll t_a$; therefore the computation of the elements of the scattering matrix even for a very large number of scattering angles (say, 1000 or so) requires only a small additional computer time.

C. Accuracy Tests

For the examination of the accuracy of this computer code, several test computations have been performed:

(1) This method was used to compute the expansion coefficients for homogeneous spherical particles, and the results obtained were compared with those obtained with the Domke method.

(2) These computations for randomly oriented homogeneous spheroids were compared with those of de Haan.[59] De Haan has used the solution by Asano and Yamamoto for spheroidal scatterers,[60] as modified by Schaefer,[61] and a method of numerical angle integrations to compute the expansion coefficients for randomly oriented homogeneous prolate spheroids ($m_r = 1.55 + 0.01i$, $a/b = 0.2499998$, $kb = 10.07937$) and oblate spheroids ($m_r = 1.53 + 0.006i$, $a/b = 1.999987$, $ka = 3$). The numerical procedure used is extensively described in Ref. 58 and is completely independent of this one, thus providing an excellent test.

(3) Some general inequalities,[5] which are to be satisfied by the expansion coefficients, were used for checking purposes.

In all the cases considered, an excellent agreement [to six decimal places in case (2)] was found.

6. DISCUSSION AND CONCLUSIONS

As was pointed out in Section 1, the expansion coefficients form a convenient and concise means of representing scattering matrices of macroscopically isotropic scattering media. Apparently, the simplest (but not the most efficient) way to compute the expansion coefficients is to use the method of numerical angle integrations in expression (2.21) and the formula [cf. Eqs. (2.15) and (2.16)]

$$\mathbf{F}^C(\theta) = \frac{1}{2\pi C_{\text{sca}}} \int_0^{2\pi} \mathrm{d}\alpha \int_0^{\pi} \mathrm{d}\beta \sin\beta \int_0^{2\pi} \mathrm{d}\gamma \mathbf{Z}^C(\theta, 0; 0, 0; \alpha\beta\gamma) \tag{6.1}$$

(see, e.g., Ref. 58). Nevertheless, I have shown in this paper that the T-matrix approach can be successfully used to evaluate all the integrals in Eqs. (2.21) and (6.1) analytically, the final expressions being rather simple and well suited for efficient computer calculations. Moreover, the method developed is numerically accurate in the above-mentioned sense: if the computational parameter $n_{\max}$ has been chosen, the T-matrix elements with $n \le n_{\max}$ are assumed to be determined precisely, and the T-matrix elements with $n > n_{\max}$ are assumed to be zero, then the accuracy of computing the expansion coefficients is limited only by round-off errors and does not depend on any additional computational parameter.

I recommend the use of this method both in multiple-scattering calculations, when only the expansion coefficients themselves have to be determined, and in single-scattering calculations, when the elements of the scattering matrix are required for a representative set of scattering angles. In the case of single-scattering calculations, the method of numerical angle integrations in Eq. (6.1) was frequently used in the literature.[35,37,38,58,62,63] Nevertheless, this method, which implies computation of the expansion coefficients before computation of the elements of the scattering matrix, seems to be much faster. For example, Barber *et al.*,[35] who used the method of numerical angle integrations and performed their calculations on a microcomputer, reported that, for a prolate-spheroidal particle with $a/b = 0.5$, $kb = 5.6$, and $m_r = 1.5$, the matrix $\mathbf{T}(A)$ was generated in 23 min, and then an overnight run was required to compute the orientationally averaged scattering matrix for 37 scattering angles. In other words, the time for computing the scattering matrix for 37 scattering angles was roughly 20 times that for computing the matrix $\mathbf{T}(A)$. For the same case but on the computer that I used, the matrix $\mathbf{T}(A)$ was generated in 19 s, the corresponding expansion coefficients were computed in 14 s, and then the orientationally averaged scattering matrix for 37 scattering angles was computed in 0.36 s. Thus the overall time for computing the scattering matrix for 37 scattering angles was even less than the time for computing the matrix $\mathbf{T}(A)$.

Also, direct comparisons of the two methods were made by solving identical scattering problems on the same ES 1061 computer. For this purpose, I used the computer program by Paramonov and Lopatin,[64] which is based on the T-matrix approach and the method of numerical angle integrations and, like this program, is written in standard FORTRAN. For the two models considered (see Subsection 5.B), I found that, in computing the orientationally averaged scattering matrix for 37 scattering angles, this program was roughly 20 times faster than that of Paramonov and Lopatin.

Finally, note that recently Schiffer[65,66] used the idea of taking an ensemble average analytically in order to compute the expansion coefficients for an ensemble of randomly oriented irregular particles. As a mathematical basis, Schiffer utilized the so-called perturbation approach,[67] which can be applied only to nearly spherically shaped particles. Schiffer's final equations have simple and transparent structure but seem not to be well suited for efficient computer calculations, since a fivefold summation has to be evaluated to compute each of the expansion coefficients. Unlike Schiffer's equations, the maximum order of summation in these formulas is only three.

APPENDIX A: GENERALIZED SPHERICAL FUNCTIONS

For integers s, p, and q, the generalized spherical functions are defined as[46]

$$P_{pq}{}^s(x) = A_{pq}{}^s(1-x)^{(p-q)/2}(1+x)^{-(p+q)/2} \times \frac{d^{s-q}}{dx^{s-q}}[(1-x)^{s-p}(1+x)^{s+p}] \quad \text{for} \quad s \ge s_* = \max(|p|, |q|) \tag{A1}$$

$$P_{pq}{}^{s}(x) = 0 \quad \text{for} \quad s < s_*, \tag{A2}$$

with

$$A_{pq}{}^{s} = \frac{(-1)^{s-p} i^{q-p}}{2^s} \left[\frac{(s+q)!}{(s-p)!(s+p)!(s-q)!} \right]^{1/2}. \tag{A3}$$

Note that

$$P_{00}{}^{s}(x) = P_s(x), \tag{A4}$$

$$P_{0q}{}^{s}(x) = i^q \left[\frac{(s-q)!}{(s+q)!} \right]^{1/2} P_s{}^{q}(x), \tag{A5}$$

where $P_s(x)$ are Legendre polynomials given by

$$P_s(x) = \frac{1}{2^s s!} \frac{\mathrm{d}^s}{\mathrm{d}x^s} (x^2 - 1)^s \tag{A6}$$

and $P_s{}^q(x)$ are associated Legendre functions given by

$$P_s{}^q(x) = \frac{(-1)^q}{2^s s!} (1 - x^2)^{q/2} \frac{\mathrm{d}^{s+q}}{\mathrm{d}x^{s+q}} (x^2 - 1)^s. \tag{A7}$$

Important properties of the generalized spherical functions are the symmetry relation

$$P_{pq}{}^{s}(x) = P_{qp}{}^{s}(x) = P_{-p-q}{}^{s}(x) = (-1)^{p+q} [P_{pq}{}^{s}(x)]^* \tag{A8}$$

and the orthogonality relation

$$\int_{-1}^{+1} \mathrm{d}x P_{pq}{}^{s}(x) P_{pq}{}^{s'}(x) = \frac{2}{2s+1} (-1)^{p+q} \delta_{ss'}. \tag{A9}$$

In practice the generalized spherical functions may be found from the recurrence relation[46]

$$\begin{aligned} s[(s+1)^2 - p^2]^{1/2}[(s+1)^2 - q^2]^{1/2} P_{pq}{}^{s+1}(x) &= (2s+1)[s(s+1)x - pq] P_{pq}{}^{s}(x) \\ &\quad - (s+1)(s^2 - p^2)^{1/2}(s^2 - q^2)^{1/2} P_{pq}{}^{s-1}(x), \end{aligned} \tag{A10}$$

with

$$P_{pq}{}^{s_*-1}(x) = 0, \tag{A11}$$

$$P_{pq}{}^{s_*}(x) = \frac{(-i)^{|p-q|}}{2^{s_*}} \left[\frac{(2s_*)!}{(|p-q|)!(|p+q|)!} \right]^{1/2} \times (1-x)^{|p-q|/2} (1+x)^{|p+q|/2}. \tag{A12}$$

APPENDIX B: CLEBSCH–GORDAN COEFFICIENTS

To calculate the Clebsch–Gordan coefficients appearing in Eqs. (4.17), (4.18), and (4.23)–(4.27), we may use the following formulas, which are given in a book by Varshalovich *et al.*[45] or can be easily derived from equations therein.

For $n' < N = \max(|n - n_1|, |m'|)$,

$$C_{nm\,n_1m'-m}{}^{n'm'} = 0. \tag{B1}$$

For $n' > N$,

$$\begin{aligned} C_{nm\,n_1m'-m}{}^{n'm'} = &\left[\frac{4n'^2(2n'+1)(2n'-1)}{(n'+m')(n'-m')(n_1-n+n')(n-n_1+n')(n+n_1-n'+1)(n+n_1+n'+1)} \right]^{1/2} \\ &\times \left\{ \frac{(2m-m')n'(n'-1) - m'n(n+1) + m'n_1(n_1+1)}{2n'(n'-1)} C_{nm\,n_1m'-m}{}^{n'-1m'} \right. \\ &\left. - \left[\frac{(n'-m'-1)(n'+m'-1)(n_1-n+n'-1)(n-n_1+n'-1)(n+n_1-n'+2)(n+n_1+n')}{4(n'-1)^2(2n'-3)(2n'-1)} \right]^{1/2} C_{nm\,n_1m'-m}{}^{n'-2m'} \right\}. \end{aligned} \tag{B2}$$

For $n' = N$, the following particular cases have to be considered:

(1) For $|n - n_1| \geq |m'|$ and $n \geq n_1$,

$$C_{nm\,n_1m'-m}{}^{n-n_1m'} = (-1)^{n_1+m'+m} \left[\frac{(n+m)!(n-m)!(2n_1)!(2n-2n_1+1)!}{(2n+1)!(n_1+m'-m)!(n_1-m'+m)!(n-n_1+m')!(n-n_1-m')!} \right]^{1/2}. \tag{B3}$$

(2) For $|n - n_1| \geq |m'|$ and $n < n_1$, we use the formula

$$C_{nm\,n_1m'-m}{}^{n_1-nm'} = C_{n_1m'-m\,nm}{}^{n_1-nm'}, \tag{B4}$$

together with Eq. (B3).

(3) For $|n - n_1| < |m'|$ and $m' \geq 0$,

$$C_{nm\,n_1m'-m}{}^{n'm'} = (-1)^{n+m} \left[\frac{(2m'+1)!(n+n_1-m')!(n+m)!(n_1+m'-m)!}{(n+n_1+m'+1)!(n-n_1+m')!(n_1-n+m')!(n-m)!(n_1-m'+m)!} \right]^{1/2}. \tag{B5}$$

(4) For $|n - n_1| < |m'|$ and $m' < 0$, we use the formula

$$C_{nm\,n_1m'-m}{}^{-m'm'} = (-1)^{n+n_1+m'} C_{n-m\,n_1m-m'}{}^{-m'-m'}, \tag{B6}$$

together with Eq. (B5).

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ERRATA

Light scattering by randomly oriented axially symmetric particles: errata

M. I. Mishchenko

Laboratory for Radiative Transfer Theory, The Main Astronomical Observatory of the Ukrainian Academy of Sciences, 252127 Kiev-127, Goloseevo, Ukraine

In Ref. 1, Eqs. (4.15), (4.16), (4.23), and (B5) should read

$$C_{-1+1} = \sum_{nmn_1} f_{nn_1} d_{1-m}{}^{n} d_{1-m0}{}^{n_1} \ldots, \tag{4.15}$$

$$C_{-1-1} = \sum_{nmn_1} f_{nn_1} d_{1m}{}^{n} d_{m-10}{}^{n_1} \ldots, \tag{4.16}$$

$$g_{00}{}^{s} = \sum_{n=1}^{\infty} \sum_{\hat{n}=\max(1,|n-s|)}^{n+s} h_{sn\hat{n}} C_{n1s0}{}^{\hat{n}1} \ldots, \tag{4.23}$$

$$C_{nm\,n_1m'-m}{}^{m'm'} = \ldots. \tag{B5}$$

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