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Notes

Expansion of tabulated scattering matrices in generalized spherical functions

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ABSTRACT

An efficient way to solve the vector radiative transfer equation for plane-parallel turbid media is to Fourier-decompose it in azimuth. This methodology is typically based on the analytical computation of the Fourier components of the phase matrix and is predicated on the knowledge of the coefficients appearing in the expansion of the normalized scattering matrix in generalized spherical functions. Quite often the expansion coefficients have to be determined from tabulated values of the scattering matrix obtained from measurements or calculated by solving the Maxwell equations. In such cases one needs an efficient and accurate computer procedure converting a tabulated scattering matrix into the corresponding set of expansion coefficients. This short communication summarizes the theoretical basis of this procedure and serves as the user guide to a simple public-domain FORTRAN program.

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1. Introduction

An efficient way of solving the vector radiative transfer equation (VRTE) for plane-parallel turbid media composed of statistically isotropic and mirror-symmetric random particles [1,2] is to Fourier-decompose the VRTE in azimuth and find each Fourier component separately (see, e.g., [3–20] and references therein). The central element of this methodology is the analytical procedure for the computation of the Fourier components of the phase matrix using the addition theorem for generalized spherical functions (GSFs). This procedure dates back to the seminal papers by Kuščer and Ribarič [21], Domke [22], Siewert [23,24], and Hovenier and van der Mee [25]. The most convenient version of this procedure based on real-valued Stokes parameters was developed by de Haan et al. [5] and summarized by Hovenier et al. [26]. Their approach is based on the underlying expansion of the corresponding normalized scattering matrix [1,2] in appropriate GSFs and is thus predicated on the knowledge of the corresponding expansion coefficients for the particle ensemble in question.

There are several numerical techniques for the explicit computation of the expansion coefficients for specific particle types based on such direct solvers of the macroscopic Maxwell equations as the Lorenz–Mie theory and the (superposition) *T*-matrix method. In particular, direct computations of the expansion coefficients bypassing the prior computation of the scattering matrix can be performed for

- monodisperse or polydisperse homogeneous and radially inhomogeneous spherical particles [27–31];
- monodisperse or polydisperse, randomly oriented homogeneous spheroids, circular cylinders, and regular 2D Chebyshev particles [30,32];
- monodisperse bispheres [33];
- clusters of separated, externally touching, and/or nested spheres [34–36].

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Several FORTRAN computer programs based on these techniques are publicly available on-line [37]. Other nonspherical shapes such as polyhedral particles, regular 3D Chebyshev particles, and 2D and 3D Gaussian random spheres can be handled using the *T*-matrix code described in [38] and also publicly available on-line [39]. Of course, these public-domain computer programs may be inapplicable to certain particle morphologies and/or size-parameter ranges. In many such cases one may be able to use the core-mantle and invariant-imbedding *T*-matrix programs described in [40–43].

Quite often however the expansion coefficients cannot be computed directly and must be determined from tabulated values of the scattering matrix elements. This happens when the scattering matrix is measured experimentally [44–48] or is computed using alternative numerical techniques such as, for example, the ray tracing (or geometrical optics) approximation [49–57], the discrete-dipole approximation [58–61], the finite-difference time-domain method [62–64], and the pseudo-spectral time domain method [65,66] (see also Refs. [67–74]). In such cases it is essential to have an efficient, accurate, and user-friendly computer procedure converting a tabulated scattering matrix into the corresponding set of expansion coefficients. The main objective of this short communication is to summarize the theoretical basis of this procedure and serve as the user guide to a simple public-domain FORTRAN program.

To make the discussion more compact, we will use throughout the terminology and notation adopted in the monographs [1,2,30]. Note that [1,30] are available on-line as PDF files at ⟨http://www.giss.nasa.gov/staff/mmishchenko/books.html⟩ as well as at https://www.researchgate.net/profile/Michael_Mishchenko.

2. Expansion of the scattering matrix in generalized spherical functions

We assume that the random particles forming a sparse turbid layer are statistically isotropic and mirror symmetric [1,2,26,30]. This means that all orientations of a particle are equally probable. Furthermore, each particle has a plane of symmetry and/or is accompanied by its mirror counterpart.

This assumption allows us to fully characterize the single-scattering properties of the particulate medium by the ensemble-averaged single-scattering albedo ϖ and so-called normalized 4×4 Stokes scattering matrix $\tilde{\mathbf{F}}(\Theta)$ with real-valued components. The latter has the well-known block-diagonal structure:

$$\tilde{\mathbf{F}}(\Theta)=\begin{bmatrix} a_1(\Theta) & b_1(\Theta) & 0 & 0 \\ b_1(\Theta) & a_2(\Theta) & 0 & 0 \\ 0 & 0 & a_3(\Theta) & b_2(\Theta) \\ 0 & 0 & -b_2(\Theta) & a_4(\Theta) \end{bmatrix}, \tag{1}$$

where $\Theta \in [0, \pi]$ is the angle between the incidence and scattering directions (i.e., the scattering angle). The (1,1) element (called the phase function) is non-negative and satisfies the normalization condition

$$\frac{1}{2}\int_0^{\pi} \mathrm{d}\Theta \ \sin\Theta \ a_1(\Theta)=1. \tag{2}$$

The elements of the normalized scattering matrix (1) can be expanded in GSFs $P^s_{mn}(\cos\Theta)$ [1,2,26,30]:

$$a_1(\Theta)=\sum_{s=0}^{s_{\max}} \alpha_1^s P^s_{00}(\cos\Theta), \tag{3}$$

$$a_2(\Theta)+a_3(\Theta)=\sum_{s=0}^{s_{\max}} (\alpha_2^s+\alpha_3^s) P^s_{22}(\cos\Theta), \tag{4}$$

$$a_2(\Theta)-a_3(\Theta)=\sum_{s=0}^{s_{\max}} (\alpha_2^s-\alpha_3^s) P^s_{2,-2}(\cos\Theta), \tag{5}$$

$$a_4(\Theta)=\sum_{s=0}^{s_{\max}} \alpha_4^s P^s_{00}(\cos\Theta), \tag{6}$$

$$b_1(\Theta)=\sum_{s=0}^{s_{\max}} \beta_1^s P^s_{02}(\cos\Theta), \tag{7}$$

$$b_2(\Theta)=\sum_{s=0}^{s_{\max}} \beta_2^s P^s_{02}(\cos\Theta), \tag{8}$$

where the upper summation limit $s_{\max}$ depends on the requisite numerical accuracy. Note that these expansions can also be written in terms of real-valued so-called Wigner *d*-functions given by

$$d^s_{mn}(\Theta)=\mathrm{i}^{n-m} P^s_{mn}(\cos\Theta) \tag{9}$$

(see [75] and Appendix F in [1]).

If the normalized scattering matrix is known beforehand, the expansion coefficients can be calculated by evaluating the following integrals:

$$\alpha_1^s=(s+\tfrac{1}{2})\int_0^{\pi} \mathrm{d}\Theta \ \sin\Theta \ a_1(\Theta)\, d^s_{00}(\Theta), \tag{10}$$

$$\alpha_2^s+\alpha_3^s=(s+\tfrac{1}{2})\int_0^{\pi} \mathrm{d}\Theta \ \sin\Theta \ [a_2(\Theta)+a_3(\Theta)]\ d^s_{22}(\Theta), \tag{11}$$

$$\alpha_2^s-\alpha_3^s=(s+\tfrac{1}{2})\int_0^{\pi} \mathrm{d}\Theta \ \sin\Theta \ [a_2(\Theta)-a_3(\Theta)]\ d^s_{2,-2}(\Theta), \tag{12}$$

$$\alpha_4^s=(s+\tfrac{1}{2})\int_0^{\pi} \mathrm{d}\Theta \ \sin\Theta \ a_4(\Theta)\, d^s_{00}(\Theta), \tag{13}$$

$$\beta_1^s=-(s+\tfrac{1}{2})\int_0^{\pi} \mathrm{d}\Theta \ \sin\Theta \ b_1(\Theta)\, d^s_{02}(\Theta), \tag{14}$$

$$\beta_2^s=-(s+\tfrac{1}{2})\int_0^{\pi} \mathrm{d}\Theta \ \sin\Theta \ b_2(\Theta)\, d^s_{02}(\Theta). \tag{15}$$

These formulas follow from Eqs. (3)–(9) and the orthogonality property of the Wigner *d*-functions [1,75].

3. Numerical integration

As we have already mentioned, in some cases the expansion coefficients can be calculated directly without computing explicitly the elements of the scattering matrix. Alternatively, one needs to evaluate the integrals (10)–(15) numerically by using a quadrature formula. By virtue of being exact for all polynomials of degree $2N_G-1$ or lower, where N_G is the number of quadrature nodes, the classical Gaussian

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