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Revisiting the Fourier expansion of Mie scattering matrices in generalized spherical functions

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ABSTRACT

Mie computations of the scattering properties of large particles are a time consuming step in the radiative transfer modeling of aerosol and clouds. Currently, there exist two methods based on the use of spherical functions for computing the Fourier moments of the phase matrix of a given spherical particle or particulate polydispersion: The first, developed over the years before being presented in a convenient form by Siewert [31], required an intermediate computation of the phase matrix over which numerical integration was performed to deliver the required Fourier components. The second, suggested by Domke [9], promised a direct computation of the Fourier moments using Wigner 3-*j* symbols.

While the former was relatively easy to implement and is thus the most commonly used to date, its numerical implementation using an arbitrary user choice of angular quadrature (NAI-1) can produce inaccurate results. Numerical integration using quadrature points as recommended by de Rooij and van der Stap [5] (NAI-2) delivers accurate results with high computational efficiency.

Domke's method enables a direct computation of the exact number of required Fourier components. However, the original manuscript contained several misprints, many of which were subsequently corrected by de Rooij and van der Stap [5]. Unfortunately, the main recurrence relationship used in Domke [9] remained uncorrected. In this paper, the corrected relationship is presented along with other minor corrections.

de Rooij and van der Stap [5] had found the straightforward application of Domke's method viable only for size parameters smaller than ~120 due to issues involving computer storage. A means of implementing the corrected Domke formalism using precomputed tabulations of Wigner 3-*j* symbols (PCW) is presented here, making it more computationally economical and applicable over much broader particle size ranges. The accuracy of PCW is only limited by machine precision. For a single particle, NAI-2 is found to be faster than PCW for size parameters greater than about 228, whereas for polydispersions over a finite range of particle sizes, PCW is found to be at least 6–8 times faster for size parameters ranging from ~0 to beyond 900. PCW thus allows for significant reduction of the computational burden associated with Mie calculations for polydispersions.

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1. Introduction

Applications such as the remote sensing of aerosol and clouds using optimized inversion methods have long been

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impeded by the time required for the accurate Mie computation of the optical properties of spherical particulate polydispersions, viz., extinction cross-section, single scattering albedo and the Fourier moments of the phase matrix, for further use in radiative transfer models [34,11,33,22,39,12,17,24,25]. This often forces the operational use of less flexible approaches such as precomputed look-up tables [23,14], or restricts the scale of the data to be analyzed to isolated case-studies [26] or synthetic sensitivity studies [26,7]. Hence, both efficiency and accuracy are critical to the choice of a method for the Fourier expansion of the phase matrix of a given particle or, more frequently, particulate polydispersion.

There exist two main methods for expanding a phase matrix in terms of its Fourier components. Usually, the scattering matrix is computed first at an appropriate number of angles. The expansion coefficients are computed by performing numerical integrations of its product with generalized spherical functions over this angular range. Theoretical work was done following this approach by Sekera [29], Kuščer and Ribarič [15], and Dave [4] and was presented in the form of "Greek matrices" (to be pre- and post-multiplied by matrices composed of generalized spherical functions computed along the directions of scattered and incident light, respectively) by Siewert [31]. While Siewert [31] demonstrated in theory that integration over the angular range of scattering was a viable means of computing the Fourier moments of the phase matrix, they did not provide a recommendation for the choice of angles to be used in the actual implementation of their method. Gauss–Legendre quadrature was generally used with an arbitrary number of roots. Sometimes, a large number of quadrature roots were avoided altogether by subdividing the full angular range into a number N_{block} of equal subintervals. A small number (usually of the same order as the number of streams employed in subsequent radiative transfer calculations, i.e., 20–40) of Gauss–Legendre quadrature roots were used within each block. We refer to this approach in the following as the first method of numerical angular interpolation (NAI-1). However, borrowing from the analysis of Domke [9], de Rooij and van der Stap [5] could specify the exact number of roots of Gauss–Legendre quadrature to be used for numerical interpolation, leading to a significant improvement in accuracy. This implementation is referred to in the following as the second method of numerical angular interpolation (NAI-2). A more detailed explanation of NAI-2 is given in Section 4.1.

Noting that the computation of the Fourier components of the phase matrix involved integrals over the product of three generalized spherical functions, Domke [9] was the first to use Wigner 3-*j* symbols [37], known from the quantum theory of angular momentum, to evaluate those integrals. This provided a powerful technique for computing the Fourier expansion coefficients directly from particle microphysical parameters without a need for the intermediate computation of the scattering matrix.

Though Domke's formalism promised significant gains in both accuracy and computational efficiency, the original manuscript by Domke [9] contained several minor but critical misprints, causing his work to be relegated to relative obscurity. Many of these misprints were corrected by de Rooij and van der Stap [5], albeit with the exception of a central recurrence relationship as well as the expression for an expansion coefficient. de Rooij and van der Stap [5] noted that while Domke's method was twice as fast as NAI-2 for small particles ($0 \le x \lesssim 120$, where $x = 2\pi r/\lambda$ is the size parameter of a particle of radius r at wavelength λ), its memory requirements become too large (< 8 GB), especially for computational capacities in 1984, to warrant fruitful use for most commonly needed size distributions. Using Domke's work to specify the exact number of angular quadrature roots required, de Rooij and van der Stap [5] concluded that NAI-2 was of more practical use than Domke's method.

This work presents in Section 4 a fully corrected and tested formalism for Domke's method, with special emphasis on the recurrence relationship misprinted in both manuscripts, [9] and de Rooij and van der Stap [5]. A derivation of the same has been provided in the Appendix. A simple alternative implementation of Domke's method (PCW) has been developed which eliminates issues involving memory usage and simultaneously improves speed by using binary files for the storage of precomputed Wigner 3-*j* symbols. As a result, we can report a six- to eight-fold improvement in computational speed compared to NAI-2 for particulate polydispersions. This has been tested for particle size parameters ranging up to $x \sim 920$.

Before proceeding to Domke's formalism, we begin in Section 2 with a brief overview of the computation of optical properties of spherical particles using Mie theory. Section 3 provides a brief overview of Siewert's formalism, before presenting Domke's corrected formalism in Section 4 and an alternate implementation circumventing memory issues in Section 4.1. Section 4.1 also includes a brief explanation of how Domke's analysis allows the exact specification of the number of quadrature roots to be used in NAI-2.

Section 5 showcases a comparison of Domke's and Siewert's formalisms based on speed and accuracy of computation for different particle sizes. The relative advantages and disadvantages of each method have been summarized.

2. Mie computations: a brief overview

Assuming a given size distribution, $\rho(r)$, of constant complex refractive index $n_r - \imath n_i$, Mie theory [35,6,38,1] provides a means of computing the complex coefficients a_n and b_n for an individual particle of size r within that distribution at a given wavelength λ, characterized by the size parameter $x = 2\pi r/\lambda$. a_n and b_n are used to compute the extinction and scattering cross-sections as functions of particle size, such that

$$C_{\text{ext}} = \frac{2\pi}{k^2}\sum_{n=1}^{\infty}(2n+1)\text{Re}(a_n+b_n) \quad \text{and}$$

$$C_{\text{scatt}} = \frac{2\pi}{k^2}\sum_{n=1}^{\infty}(2n+1)\{|a_n|^2+|b_n|^2\}, \tag{1}$$

where $k = 2\pi/\lambda$ is the wave number. The scattering matrix $\mathbf{F}(\xi)$ describes the distribution of light scattered by the