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

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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, 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, promised a direct computation of the Fourier moments using Wigner3-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 (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. Unfortunately, the main recurrence relationship used in Domke remained uncorrected. In this paper, the corrected relationship is presented along with other minor corrections. de Rooij and van der Stap had found the straightforward application of Domke's method viable only for size parameters smaller than $\sim$120 due to issues involving computer storage. A means of implementing the corrected Domke formalism using precomputed tabulations of Wigner3-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 atleast 6–8 times faster for size parameters ranging from $\sim$0 to beyond 900. PCW thus allows for significant reduction of the computational burden associated with Mie calculations for polydispersions.