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Symmetry relations for the Mueller scattering matrix integrated over the azimuthal angle

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ABSTRACT

Explicit symmetry relations for azimuthal Fourier components of the Mueller scattering matrix were derived as implications of particular scatterer symmetries. Several types of the latter were considered, including plane symmetries and second- and fourth-order rotational symmetries around the *z*-axis. Depending on the particular symmetry the integrals of the Mueller matrix over the azimuthal angle either vanish or equal the ones computed over the reduced angular range. Derived relations provide an independent test for any computer code that computes these integrals, which was illustrated by the discrete-dipole-approximation simulations for a number of test particles. Moreover, these relations can be used to reduce the time for computing these integrals for a symmetric particle by several times, which is relevant for several specific applications.

1. Introduction

Symmetries are fundamental to the light-scattering theory. They allow one to solve the light-scattering problem for a wide variety of particle shapes: from the most symmetric shape, a sphere [1], to more complex shapes with finite-order symmetries [2,3]. Another kind of symmetry is that of the computed results, in particular, of the Mueller matrix elements [4]. Such symmetries have smaller direct utility, since the scattering problem has to be solved beforehand. However, they are more general, applying in some form to almost all kinds of scatterers, and constitute an independent test for both simulation results, e.g. [5–7], and experimental measurements of light-scattering [8,9]. A comprehensive treatment of Mueller matrix symmetry for single particles and ensembles in fixed and random orientations was performed by van de Hulst [10]. It was further extended by Hovenier and van der Mee [11] with emphasis on practical tests for simulation or experimental results. Specific tests for horizontally oriented particles were also derived [12].

In this paper I consider the Mueller matrix elements integrated over the whole range of the azimuthal scattering angle. To the best of my knowledge, applications of light-scattering symmetries to such integrals have never been considered before, except for a special case in [13]. Specifically, I consider the following integrals:

$$c_{ij}^{m}(\theta)=\frac{1}{2\pi}\int_{0}^{2\pi}\mathrm{d}\varphi S_{ij}(\theta,\varphi)\cos(m\varphi),$$
$$s_{ij}^{m}(\theta)=\frac{1}{2\pi}\int_{0}^{2\pi}\mathrm{d}\varphi S_{ij}(\theta,\varphi)\sin(m\varphi), \qquad (1)$$

where m is an integer, θ and φ are the polar and azimuthal scattering angles respective to the incident direction, that is further assumed to be along the positive z-axis. S_{ij} is the Mueller matrix element, defined relative to the scattering plane, containing the incident and scattered direction [4]. In particular, if a particle is symmetric with respect to any rotation over the z-axis, S_{ij} is independent of φ. The integrals, described by Eq. (1), are relevant to flow cytometry. In particular, almost any flow cytometer

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measures forward scattering of single particles in flow, as an integral of the scattering intensity over a certain solid angle near the forward direction. In some configurations azimuthally-symmetric ring detectors are used [14,15], hence the signal can be expressed in terms of $c_{ij}^0(\theta)$. Sometimes several forward-scattering signals for different ranges of θ are used [16], and similar configurations are employed in optical particle sizers [17].

A variation of flow cytometry, scanning flow cytometry (SFC) [18,19], makes even larger use of integrals in Eq. (1). The central part of the SFC optical system is a spherical mirror, symmetric over the incident laser beam [18]. Thus, all measured signals are integrated over the azimuthal angle. Specific expressions depend upon the polarizing optical elements before and after the measured particle [19]. For example, the latest generation of the SFC measures the following signal [20]:

$$I(\theta)=\int_0^{2\pi}\mathrm{d}\varphi[S_{11}(\theta,\varphi)+S_{14}(\theta,\varphi)+(S_{21}(\theta,\varphi)+S_{24}(\theta,\varphi))\cos 2\varphi-(S_{31}(\theta,\varphi)+S_{34}(\theta,\varphi))\sin 2\varphi] \quad (2)$$

in a wide range of θ. It can be expressed in terms of $c_{ij}^0(\theta)$, $c_{ij}^2(\theta)$, and $s_{ij}^2(\theta)$, while expressions, involving $c_{ij}^4(\theta)$ and $s_{ij}^4(\theta)$, may occur in future versions of the SFC [19]. That is why the discrete-dipole-approximation (DDA, [21]) code ADDA [22] includes functionality to automatically calculate $c_{ij}^{0,2,4}(\theta)$ and $s_{ij}^{2,4}(\theta)$ for a single particle of arbitrary shape and composition.

Another possible utility of Eq. (1) comes from the following combinations:

$$a_{ij}^m(\theta)=\frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\varphi S_{ij}(\theta,\varphi)\exp(\mathrm{i}m\varphi)=c_{ij}^m(\theta)+\mathrm{i}s_{ij}^m(\theta), \quad (3)$$

which can be considered as Fourier harmonics of the 2D light-scattering patterns (LSPs). Moreover, it is an intermediate step to obtain expansion coefficients of $S_{ij}(\theta,\varphi)$ in terms of the scalar spherical harmonics $Y_{lm}(\theta,\varphi)$

$$b_{ij}^{lm}=\oint \mathrm{d}\Omega S_{ij}(\theta,\varphi)Y_{lm}^*(\theta,\varphi)=N_l\int_0^{\pi}\mathrm{d}\theta a_{ij}^{m*}(\theta)d_{m0}^l(\theta) \quad (4)$$

where $d_{m0}^l(\theta)$ is the Wigner d-function, N_l the normalization constant, and $*$ denotes complex conjugation (see e.g. [23]). Coefficients $a_{ij}^m(\theta)$ and b_{ij}^{lm} can be used to compress 2D LSPs calculated on a grid of scattering angles into a (smaller) set of numbers. Moreover, these coefficients can potentially be directly computed, without $S_{ij}(\theta,\varphi)$ themselves, by some of the light-scattering methods, such as the T-matrix method [23].

The goal of this paper is to analyze the effect of certain particle symmetries on Eqs. (1) and (3) both to derive tests for verification of numerical simulations and/or experimental measurements and to improve the brute-force computation of these integrals by the light-scattering codes. To verify theoretical conclusions I also present several sample simulations with the DDA.

2. Symmetry of a particle in a fixed orientation

Keeping the SFC applications in mind, I limit myself to the symmetries which are relevant for a fixed value of θ. This generally omits the reciprocity, rotational symmetry around other than the z-axis, and symmetry planes not containing the z-axis. However, the following trivial relations always hold:

$$c_{ij}^m(\theta)=c_{ij}^{-m}(\theta),\ s_{ij}^m(\theta)=-s_{ij}^{-m}(\theta),\ a_{ij}^m(\theta)=a_{ij}^{-m*}(\theta). \quad (5)$$

Let me further consider a particle that is symmetric over the plane $\varphi=\varphi_0$, which scatters light incident along the z-axis. Compare two scattering directions characterized by angles $(\theta,\varphi_0+\varphi)$ and $(\theta,\varphi_0-\varphi)$. Let us denote the amplitude scattering matrices in these directions by S_a and S'_a and Mueller matrices—by S and S' respectively. Scattering configurations $(\theta,\varphi_0+\varphi)$ and $(\theta,\varphi_0-\varphi)$ are completely mirror-symmetric, for which van de Hulst showed [10] that amplitude matrices differ only in signs of the off-diagonal elements:

$$S'_a=\begin{pmatrix} S'_2 & S'_3 \\ S'_4 & S'_1 \end{pmatrix}=\begin{pmatrix} S_2 & -S_3 \\ -S_4 & S_1 \end{pmatrix} \quad (6)$$

employing transformation of the amplitude matrix into the Mueller one (see e.g. [4]) and Eq. (6) one may easily obtain that S and S' differ only in signs of the off-block-diagonal elements:

$$S'=\begin{pmatrix} S'_{11} & S'_{12} & S'_{13} & S'_{14} \\ S'_{21} & S'_{22} & S'_{23} & S'_{24} \\ S'_{31} & S'_{32} & S'_{33} & S'_{34} \\ S'_{41} & S'_{42} & S'_{43} & S'_{44} \end{pmatrix}=\begin{pmatrix} S_{11} & S_{12} & -S_{13} & -S_{14} \\ S_{21} & S_{22} & -S_{23} & -S_{24} \\ -S_{31} & -S_{32} & S_{33} & S_{34} \\ -S_{41} & -S_{42} & S_{43} & S_{44} \end{pmatrix}, \quad (7)$$

or equivalently

$$S_{ij}(\theta,\varphi_0+\varphi)=S_{ij}(\theta,\varphi_0-\varphi)\times\begin{cases} 1, & \{i,j\}\in \mathrm{BD} \\ -1, & \{i,j\}\notin \mathrm{BD} \end{cases}, \quad (8)$$

where BD stands for block-diagonal, i.e. either both $i,j\le 2$ or both $i,j\ge 3$. This corollary of the existence of plane of symmetry was also derived in [12]. Splitting the integration range in Eq. (3) into $[\varphi_0,\varphi_0+\pi]$ and $[\varphi_0+\pi,\varphi_0+2\pi]$ and using Eq. (8) for the second range, one can obtain:

$$a_{ij}^m(\theta)=\frac{\exp(\mathrm{i}m\varphi_0)}{\pi}\int_{\varphi_0}^{\varphi_0+\pi}\mathrm{d}\varphi S_{ij}(\theta,\varphi)\times\begin{cases} \cos[m(\varphi-\varphi_0)], & \{i,j\}\in \mathrm{BD} \\ \mathrm{i}\sin[m(\varphi-\varphi_0)], & \{i,j\}\notin \mathrm{BD} \end{cases}, \quad (9)$$

which, in turn, implies that

$$c_{ij}^m(\theta)=s_{ij}^m(\theta)\times\begin{cases} \cot(m\varphi_0), & \{i,j\}\in \mathrm{BD} \\ -\tan(m\varphi_0), & \{i,j\}\notin \mathrm{BD} \end{cases}. \quad (10)$$

Symmetry implications are especially simple for $\varphi_0=0$, i.e. for the symmetry with respect to the xz-plane (Fig. 1(a)):

$$c_{ij}^m(\theta)=\begin{cases} \frac{1}{\pi}\int_0^{\pi}\mathrm{d}\varphi S_{ij}(\theta,\varphi)\cos(m\varphi), \{i,j\}\in \mathrm{BD}; \\ 0,\ \{i,j\}\notin \mathrm{BD}. \end{cases} \quad (11)$$

$$s_{ij}^m(\theta)=\begin{cases} 0,\ \{i,j\}\in \mathrm{BD}; \\ \frac{1}{\pi}\int_0^{\pi}\mathrm{d}\varphi S_{ij}(\theta,\varphi)\sin(m\varphi),\ \{i,j\}\notin \mathrm{BD} \end{cases} \quad (12)$$

Eqs. (11) and (12) allow one to reduce the number of calculations for averaging Mueller matrix elements over the azimuthal angle (with different weighting functions) – half of the integrals need not to be evaluated at all, while the rest – only require evaluation through half of the azimuthal range.