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Far-field Lorenz–Mie scattering in an absorbing host medium: Theoretical formalism and FORTRAN program

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ABSTRACT

In this paper we make practical use of the recently developed first-principles approach to electromagnetic scattering by particles immersed in an unbounded absorbing host medium. Specifically, we introduce an actual computational tool for the calculation of pertinent far-field optical observables in the context of the classical Lorenz–Mie theory. The paper summarizes the relevant theoretical formalism, explains various aspects of the corresponding numerical algorithm, specifies the input and output parameters of a FORTRAN program available at https://www.giss.nasa.gov/staff/mmishchenko/Lorenz-Mie.html, and tabulates benchmark results useful for testing purposes. This public-domain FORTRAN program enables one to solve the following two important problems: (i) simulate theoretically the reading of a remote well-collimated radiometer measuring electromagnetic scattering by an individual spherical particle or a small random group of spherical particles; and (ii) compute the single-scattering parameters that enter the vector radiative transfer equation derived directly from the Maxwell equations.

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1. Introduction

Electromagnetic scattering by particles immersed in an unbounded absorbing host medium has been the subject of active yet somewhat controversial research [1–26]. Most of the controversy had stemmed from the enduring desire to preserve the conventional notions of the optical cross sections introduced in the context of electromagnetic scattering in a nonabsorbing host [27–29] as well as their traditional usage in the phenomenological radiative transfer equation [30–50]. The resolution of this controversy has come from (i) relying on the first-principles derivation of the entire theoretical formalism (including the radiative transfer theory) directly from the macroscopic Maxwell equations [21–23], and (ii) the realization that in the context of classical macroscopic electromagnetics, the introduction of an optical observable is only meaningful if it addresses one or both of the following two fundamental problems [51,52]:

- model theoretically the reading of a specific detector of electromagnetic radiation; and
- quantify the electromagnetic energy budget of a finite volume of space.

In the final analysis, it is the practical solution of these problems that demonstrates what theoretical notions are contrived and what optical observables emerge naturally and thereby serve as legitimate components of the scattering formalism.

The objective of this paper is to apply the main results of Refs. [21–23] to the development of a practical computational tool for the calculation of relevant far-field optical observables in the framework of the classical Lorenz–Mie theory of electromagnetic scattering by a homogeneous spherical particle embedded in an unbounded absorbing host medium [53]. We summarize all pertinent formulas, describe in detail the corresponding numerical algorithm, list the input and output parameters of the resulting public-domain FORTRAN program available at https://www.giss.nasa.gov/staff/mmishchenko/Lorenz-Mie.html, and tabulate benchmark numerical results useful for testing purposes. The quantities generated by this program can be used to solve the following two problems of actual practical significance:

1. quantify the reading of a remote polarization-sensitive well-collimated radiometer measuring electromagnetic scattering by an individual spherical particle or a small random group of spherical particles; and
2. compute the single-scattering parameters that enter the vector radiative transfer equation derived in Refs. [22,23] directly from the macroscopic Maxwell equations.

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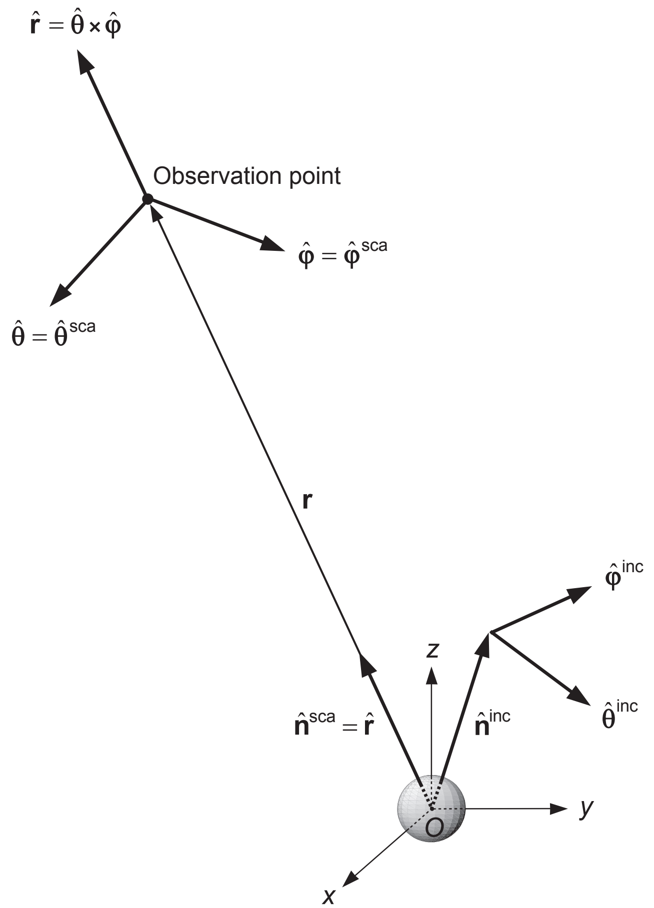

Fig. 1. Far-field electromagnetic scattering by a homogeneous spherical particle embedded in a homogeneous absorbing host medium.

Since this paper is intended, in particular, to serve as a detailed user guide to an actual computer program, we have tried to make it maximally self-contained. This explains the inclusion of more than 100 formulas, some of which are well known.

2. Far-field frequency-domain formalism

Consistent with Refs. [28,29,53], in this paper we assume the $\exp(-\mathrm{i}\omega t)$ time-harmonic dependence of all electromagnetic fields, where $\mathrm{i} = (-1)^{1/2}$, ω is the angular frequency, and t is time. Consider a fixed homogeneous spherical object embedded in an infinite, homogeneous, linear, isotropic, nonmagnetic, and, in general, absorbing host medium (see Section 9.25 of Ref. [53]). We assume that the object is made of an isotropic, linear, and nonmagnetic material. The central point O of the spherical object serves as the origin of the laboratory coordinate system and as the common origin of all position vectors $\mathbf{r}$ (Fig. 1). Let ε_1 and ε_2 be the complex-valued permittivities of the host medium and the scattering object, respectively, and μ_0 be the (real-valued) permeability of a vacuum. Then the wave numbers of the host and the object are given, respectively, by

$$k_1 = k_1' + \mathrm{i}k_1'' = \omega\sqrt{\varepsilon_1\mu_0} \tag{1}$$

and

$$k_2 = k_2' + \mathrm{i}k_2'' = \omega\sqrt{\varepsilon_2\mu_0}, \tag{2}$$

where $k'_1 > 0$, $k''_1 \geq 0$, $k'_2 > 0$, and $k''_2 \geq 0$. In practice, it is convenient to define the scattering problem in terms of the wavelength in a vacuum, λ, and the complex refractive indices of the host, m_1, and the object, m_2, given, respectively, by

$$m_1 = m_1' + \mathrm{i}m_1'' = \sqrt{\frac{\varepsilon_1}{\varepsilon_0}} \tag{3}$$

and

$$m_2 = m_2' + \mathrm{i}m_2'' = \sqrt{\frac{\varepsilon_2}{\varepsilon_0}}, \tag{4}$$

where ε_0 is the electric permittivity of a vacuum. Then

$$\omega = \frac{2\pi c}{\lambda}, \tag{5}$$

$$k_1 = \frac{2\pi m_1}{\lambda}, \tag{6}$$

and

$$k_2 = \frac{2\pi m_2}{\lambda}, \tag{7}$$

where

$$c = \frac{1}{\sqrt{\varepsilon_0\mu_0}} \tag{8}$$

is the speed of light in a vacuum.

To allow for an unambiguous definition of the Stokes parameters, let us further assume the incident field to be a *homogeneous* (or *uniform* [54]) plane electromagnetic wave propagating in the direction of the unit vector $\hat{\mathbf{n}}^{\mathrm{inc}}$ and given by

$$\mathbf{E}^{\mathrm{inc}}(\mathbf{r}) = \exp\left(\mathrm{i}k_1\hat{\mathbf{n}}^{\mathrm{inc}}\cdot\mathbf{r}\right)\mathbf{E}_0^{\mathrm{inc}}, \quad \mathbf{E}_0^{\mathrm{inc}}\cdot\hat{\mathbf{n}}^{\mathrm{inc}} = 0, \tag{9}$$

where $\mathbf{r}$ is the position vector of the observation point (Fig. 1). Note that $\mathbf{E}_0^{\mathrm{inc}}$ is the electric field at the origin of the laboratory coordinate system. In the far zone of the object, the scattered field becomes an outgoing transverse spherical wave given by [21]

$$\begin{aligned}\mathbf{E}^{\mathrm{sca}}(\mathbf{r}) &\underset{r\to\infty}{\to} \exp(-k''_1 r)\frac{\exp(\mathrm{i}k'_1 r)}{r}\mathbf{E}_1^{\mathrm{sca}}(\hat{\mathbf{n}}^{\mathrm{sca}})\\ &= \exp(-k''_1 r)\frac{\exp(\mathrm{i}k'_1 r)}{r}\overleftrightarrow{A}(\hat{\mathbf{n}}^{\mathrm{sca}},\hat{\mathbf{n}}^{\mathrm{inc}})\cdot\mathbf{E}_0^{\mathrm{inc}}.\end{aligned} \tag{10}$$

Here, $r = |\mathbf{r}|$ is the distance from the origin; $\hat{\mathbf{n}}^{\mathrm{sca}} = \hat{\mathbf{r}} = \mathbf{r}/r$ is the unit vector in the scattering direction; and $\overleftrightarrow{A}(\hat{\mathbf{n}}^{\mathrm{sca}},\hat{\mathbf{n}}^{\mathrm{inc}})$ is the scattering dyadic such that

$$\hat{\mathbf{n}}^{\mathrm{sca}}\cdot\overleftrightarrow{A}(\hat{\mathbf{n}}^{\mathrm{sca}},\hat{\mathbf{n}}^{\mathrm{inc}}) = \mathbf{0} \tag{11}$$

and

$$\overleftrightarrow{A}(\hat{\mathbf{n}}^{\mathrm{sca}},\hat{\mathbf{n}}^{\mathrm{inc}})\cdot\hat{\mathbf{n}}^{\mathrm{inc}} = \mathbf{0}, \tag{12}$$

where $\mathbf{0}$ is a zero vector. Importantly, the angular and radial dependencies on the right-hand side of Eq. (10) are completely separated, so that the scattering dyadic is independent of r. The scattering dyadic has the dimension of length.

The total electric field at a far-field observation point is the sum of the incident and scattered fields:

$$\begin{aligned}\mathbf{E}(\mathbf{r}) &= \exp(\mathrm{i}k_1\hat{\mathbf{n}}^{\mathrm{inc}}\cdot\mathbf{r})\mathbf{E}_0^{\mathrm{inc}} + \exp(-k''_1 r)\\ &\quad\times\frac{\exp(\mathrm{i}k'_1 r)}{r}\overleftrightarrow{A}(\hat{\mathbf{n}}^{\mathrm{sca}},\hat{\mathbf{n}}^{\mathrm{inc}})\cdot\mathbf{E}_0^{\mathrm{inc}}.\end{aligned} \tag{13}$$

It is straightforward to derive that the total far-field magnetic field is given by

$$\begin{aligned}\mathbf{H}(\mathbf{r}) &= \exp(\mathrm{i}k_1\hat{\mathbf{n}}^{\mathrm{inc}}\cdot\mathbf{r})\frac{k_1}{\omega\mu_0}\hat{\mathbf{n}}^{\mathrm{inc}}\times\mathbf{E}_0^{\mathrm{inc}} + \exp(-k''_1 r)\\ &\quad\times\frac{\exp(\mathrm{i}k'_1 r)}{r}\frac{k_1}{\omega\mu_0}\hat{\mathbf{n}}^{\mathrm{sca}}\times[\overleftrightarrow{A}(\hat{\mathbf{n}}^{\mathrm{sca}},\hat{\mathbf{n}}^{\mathrm{inc}})\cdot\mathbf{E}_0^{\mathrm{inc}}].\end{aligned} \tag{14}$$