Journal of Quantitative Spectroscopy & Radiative Transfer 123 (2013) 17–22

Contents lists available at SciVerse ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

journal homepage: www.elsevier.com/locate/jqsrt

A numerical combination of extended boundary condition method and invariant imbedding method applied to light scattering by large spheroids and cylinders

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ARTICLE INFO

Article history:
Received 16 October 2012
Received in revised form
29 November 2012
Accepted 30 November 2012
Available online 29 January 2013

Keywords:
Light scattering
T-matrix
Extended boundary condition method
Invariant imbedding method

ABSTRACT

The extended boundary condition method (EBCM) and invariant imbedding method (IIM) are two fundamentally different T-matrix methods for the solution of light scattering by nonspherical particles. The standard EBCM is very efficient but encounters a loss of precision when the particle size is large, the maximum size being sensitive to the particle aspect ratio. The IIM can be applied to particles in a relatively large size parameter range but requires extensive computational time due to the number of spherical layers in the particle volume discretization. A numerical combination of the EBCM and the IIM (hereafter, the EBCM+IIM) is proposed to overcome the aforementioned disadvantages of each method. Even though the EBCM can fail to obtain the T-matrix of a considered particle, it is valuable for decreasing the computational domain (i.e., the number of spherical layers) of the IIM by providing the initial T-matrix associated with an iterative procedure in the IIM. The EBCM+IIM is demonstrated to be more efficient than the IIM in obtaining the optical properties of large size parameter particles beyond the convergence limit of the EBCM. The numerical performance of the EBCM+IIM is illustrated through representative calculations in spheroidal and cylindrical particle cases.

1. Introduction

In a turbid medium, electromagnetic wave interactions with dielectric particles create many interesting physical problems. The light scattering by ice crystals and aerosols in the atmosphere, by particulates in oceanic waters, and by cells in biophysical systems are some of the better-known examples [1]. The particles are, more often than not, nonspherical and the particle size can range from a few microns to hundreds or even thousands of microns (e.g., large ice crystals). A common research topic regarding light–particle interaction system is to use Maxwell's equations to obtain the single-scattering properties of nonspherical particles in a wide range of particle size parameters (ratio of particle size to incident wavelength), which include Rayleigh, resonant, or geometric optics regimes. The T-matrix methods are among the most accurate of the various computational methods and can obtain the widest size parameter range (up to geometric optics regimes) of particle optical properties for axially symmetric particles, e.g., spheroids or circular cylinders.

Few numerical methods are available to compute the T-matrix in the T-matrix formulation of light scattering. The extended boundary condition method (EBCM), or Waterman's T-matrix method, initially proposed by

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http://dx.doi.org/10.1016/j.jqsrt.2012.11.033

Waterman [2,3] and later developed by Barber and Hill [4], Mishchenko et al. [5], and others has been popular in solving light scattering by nonspherical axially symmetric particles. In principle, the EBCM is applicable to particles of arbitrary shapes and sizes; however, the method can suffer from computational issues (e.g., [6]). One computational issue limiting the applicability of the EBCM is the ill-condition problem in inverting the so-called Q-matrix. Several attempts to circumvent or partially solve the ill-condition problem involved in the standard EBCM have been reported in the literature. For example, Mishchenko and Travis [7] found that the numerical implementation of the EBCM with extended precision variables instead of that with double precision variables could increase the maximum convergent size parameter by factors of two or three; Doicu et al. [8] developed the nullfield method with discrete sources to combine the advantages of the null field method and the method of discrete sources; Yan et al. [9] transformed the long circular cylinder single-body scattering problem into a "multi-body" scattering problem in terms of small cylinders; Kahnert and Rother [10] proposed a perturbation approach to obtain the Q-matrix inversion, and, Kahnert [11] reported that group theory could solve the numerical-ill condition problem using irreducible representations of finite groups. Further efforts to ameliorate EBCM numerical convergence problems are documented in Refs. [12–14].

Unlike the EBCM-related T-matrix methods, based on surface-integration equations, the invariant imbedding method (IIM) originates from an electromagnetic volume integral equation and iteratively obtains the T-matrix from the origin of the coordinate system by growing the scattering volume incrementally in a shell-by-shell manner. Johnson [15] first applied the IIM to solve the electromagnetic scattering by dielectric particles, and the present authors revisited the IIM based on state-of-the-art numerical implementation [16]. Numerical results show that the IIM is applicable to particles with large size parameters and extreme aspect ratios. In comparison with the EBCM, the IIM is less efficient because of the potentially large number of differential spherical shells required to discretize large sized particle volumes. To reduce the IIM computational time, the starting point of the iterative procedure can be chosen at the inscribed sphere rather than the origin, and the T-matrix of the inscribed sphere can be easily obtained by the separation of variables (SOV) method (i.e., the Lorenz–Mie theory). A combination of the SOV and the IIM (hereafter, SOV+IIM) applied to large spheroids and cylinders beyond the EBCM's convergence limit has been reported by Bi et al. [16]. Note, although the IIM or IIM+SOV is applicable to cases that the EBCM can handle, the EBCM is much faster and, thus, is recommended for practical numerical calculations.

Below we explore a numerical combination of the EBCM and the IIM to solve the light scattering by nonspherical particles in the regions where the EBCM is inapplicable. The basic principle is to employ the EBCM to further increase the starting position of the iterative procedures (see Section 2) involved in the IIM. Although the EBCM is unable to obtain the T-matrix of the whole particle, the T-matrix is calculated for a partial volume of the particle whose surface is treated as a new initial position in the IIM. Some modifications to the EBCM have been reported in the literature, but we choose to only consider the standard EBCM outlined by Mishchenko et al. [5]. For simplicity, we use the EBCM code with double precision variables and LU-factorization. Furthermore, we only consider spheroids and cylinders, although the EBCM+IIM can be applied to other geometries if the computational domains of the EBCM and the IIM are properly identified.

The paper is organized into four sections: Section 2 is a description of the EBCM and the EBCM+IIM; Section 3 discusses some representative numerical results; and, Section 4 is a summary of our study.

2. Method

Fig. 1 is a schematic diagram of the EBCM+IIM applied to spheroids and cylinders. The EBCM is applied to the geometry within a sphere of radius r_0 whose surface is composed of patches on the sphere and the considered nonspherical particle. According to the EBCM, the T-matrix at r_0 is given by [5]

$$\overline{\overline{\mathbf{T}}}(r_0) = -(\mathrm{Rg}\overline{\overline{\mathbf{Q}}})\overline{\overline{\mathbf{Q}}}^{-1}. \tag{1}$$

In the framework of the IIM, the T-matrix of the p-layer inhomogeneous spherical particle is given by [15,16]

$$\overline{\overline{\mathbf{T}}}(r_p) = \overline{\overline{\mathbf{Q}}}_{11}(r_p) + [\overline{\overline{\mathbf{I}}} + \overline{\overline{\mathbf{Q}}}_{12}(r_p)][\overline{\overline{\mathbf{I}}} - \overline{\overline{\mathbf{T}}}(r_{p-1})\overline{\overline{\mathbf{Q}}}_{22}(r_p)]^{-1}\overline{\overline{\mathbf{T}}}(r_{p-1})[\overline{\overline{\mathbf{I}}} + \overline{\overline{\mathbf{Q}}}_{21}(r_p)], \tag{2}$$

where $\overline{\overline{\mathbf{T}}}(r_{p-1})$ is the T-matrix at the shell of r_{p-1}, where p is ranging from 1 to N (r_N indicates the circumscribed spherical surface). For brevity, the definitions of the quantities $\mathrm{Rg}\overline{\overline{\mathbf{Q}}}$, $\overline{\overline{\mathbf{Q}}}$ in Eq. (1) and $\overline{\overline{\mathbf{Q}}}_{11}$, $\overline{\overline{\mathbf{Q}}}_{12}$, $\overline{\overline{\mathbf{Q}}}_{21}$, and $\overline{\overline{\mathbf{Q}}}_{22}$ in Eq. (2) will not be addressed and the reader is referred to Refs. [5,16]. Note that r_1 is equal to r_0 and indicates the same spherical surface.

The EBCM+IIM combination is based on two premises: (1) the EBCM fails at the size parameter of the concerned particle; and, (2) the EBCM works for a partial volume of spheroids and cylinders within the sphere of radius r, which is most often the case, because the maximum convergence size parameter for a near-spherical particle is relatively larger than that of a particle with an extreme aspect ratio. In addition to the fact that the EBCM+IIM can be applied to large sized particles, two byproducts are available: (1) the refractive index of the particle volume shaded in Fig. 1 whose T-matrix is computed by the EBCM can be different from the refractive index of the remaining volume where the IIM is involved in the computation; and, (2) the EBCM+IIM yields the optical properties of a series of nonspherical particles created by the intersection between a spheroid or a cylinder and multiple spherical surfaces specified by r_p ($0 \le p \le N$).

In the numerical computations, the intersection curve of spherical shells and the considered nonspherical particles must be identified. To be more specific, the range of the polar angle cosine $[\mu_1, \mu_2]$ that indicates the spherical surface within the dielectric particle is required (see e.g.,