Journal of Quantitative Spectroscopy & Radiative Transfer 116 (2013) 169–183

Contents lists available at SciVerse ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

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

Efficient implementation of the invariant imbedding T-matrix method and the separation of variables method applied to large nonspherical inhomogeneous particles

Lei Bi [a], Ping Yang [a,*], George W. Kattawar [b], Michael I. Mishchenko [c]

[a] Department of Atmospheric Sciences, Texas A&M University, College Station, TX 77843, USA
[b] Department of Physics & Astronomy, Texas A&M University, College Station, TX 77843, USA
[c] NASA Goddard Institute for Space Studies, 2880 Broadway, New York, NY 10025, USA

ARTICLE INFO

Article history:
Received 31 August 2012
Received in revised form
6 November 2012
Accepted 8 November 2012
Available online 23 November 2012

Keywords:
Invariant imbedding method
Separation of variables method
T-matrix

ABSTRACT

Three terms, "Waterman's T-matrix method", "extended boundary condition method (EBCM)", and "null field method", have been interchangeable in the literature to indicate a method based on surface integral equations to calculate the T-matrix. Unlike the previous method, the invariant imbedding method (IIM) calculates the T-matrix by the use of a volume integral equation. In addition, the standard separation of variables method (SOV) can be applied to compute the T-matrix of a sphere centered at the origin of the coordinate system and having a maximal radius such that the sphere remains inscribed within a nonspherical particle. This study explores the feasibility of a numerical combination of the IIM and the SOV, hereafter referred to as the IIM+SOV method, for computing the single-scattering properties of nonspherical dielectric particles, which are, in general, inhomogeneous. The IIM+SOV method is shown to be capable of solving light-scattering problems for large nonspherical particles where the standard EBCM fails to converge. The IIM+SOV method is flexible and applicable to inhomogeneous particles and aggregated nonspherical particles (overlapped circumscribed spheres) representing a challenge to the standard superposition T-matrix method. The IIM+SOV computational program, developed in this study, is validated against EBCM simulated spheroid and cylinder cases with excellent numerical agreement (up to four decimal places). In addition, solutions for cylinders with large aspect ratios, inhomogeneous particles, and two-particle systems are compared with results from discrete dipole approximation (DDA) computations, and comparisons with the improved geometric-optics method (IGOM) are found to be quite encouraging.

1. Introduction

In various scientific disciplines (bio-optics, photonics, astrophysics, and atmospheric radiative transfer and remote sensing), accurate and efficient computations of the optical properties of dielectric particles are often required. The Lorenz–Mie theory and its modifications [1–5] applicable to homogenous or layered spheres cannot be used to compute the optical properties of morphologically complex particulates. Great strides have been made toward accurate simulations of the scattering of light by particles of various shapes and/or chemical compositions, but, although a variety of methods have been developed [6,7], each method has its own strengths and weaknesses. For example, the full-electromagnetic wave methods of solving Maxwell's equations become inefficient or even inapplicable when the particle size is excessively large,

* Correspondence to: Department of Atmospheric Sciences, Texas A&M University, TAMU-3150, College Station, TX 77843, USA.
E-mail address: pyang@tamu.edu (P. Yang).

0022-4073/$ - see front matter © 2012 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.jqsrt.2012.11.014

whereas the semi-empirical geometric-optics method is applicable to large particles but fails for small particles when the “ray” concept is not valid. Tremendous effort has been expended to broaden the computational domain of the existing light scattering computational methods e.g., [8–16] and to gain a better understanding of the single-scattering properties of nonspherical particles with size parameters ranging from the Rayleigh to geometric-optics regimes.

Waterman's T-matrix method (TMM) [17,18] is an accurate and powerful tool capable of yielding a highly accurate numerical solution for the scattering of light by nonspherical particles [19–22]. In the literature, the technique is sometimes referred to as either the extended boundary condition method (EBCM) or the null field method. In contrast to many numerical techniques that explicitly consider the particle orientation and polarization state of the incident light in the simulations [23–28], the TMM calculates the T-matrix, a quantity independent of the propagation direction, incident light polarization state, and the scattering direction, and which allows for efficient computation of the orientation-averaged optical properties [29]. The conceptual framework of the TMM has subsequently been expanded to handle composite particles, layered particles, and more complicated scattering cases e.g., [21,22,30–33]. These developments have demonstrated the EBCM to be just one possible path to compute the T-matrix of the scattering object. Some attempts [8,34–37] to improve the limited applicability of the EBCM to certain particles have focused on numerical instability, convergence issues, and loss of precision; however, the maximum size parameter value for a convergent EBCM solution strongly depends on the particle shape. Specific details of various TMM implementations and relevant applications can be found in the texts [20–22] and a reference database [38,39]. The cumulative body of relevant research has made the TMM one of the most widely used approaches to obtain highly accurate numerical optical properties of morphologically complex particles with moderate aspect ratios and size parameters ranging from zero to $\sim$200.

As mentioned, the T-matrix, relating the incident to the scattered field expansions in vector spherical wave functions (VSWFs), can be computed from several alternative approaches in addition to the EBCM. Johnson [40] derived the T-matrix from the standard electromagnetic volume integral equation (VIE) and developed an invariant imbedding method (IIM) to iteratively calculate the T-matrix. Schulz et al. [41] obtained the T-matrix of spheroids based on the separation of variables (SOV) method in spheroidal coordinates. A discrete dipole moment method to calculate the T-matrix was developed by Mackowski [42], while Loke et al. [43] incorporated the discrete dipole approximation (DDA) into the point-matching method to calculate the T-matrix. A superposition T-matrix method (STMM) for multiple-sphere clusters developed by Peterson and Ström [30] and Mackowski and Mishchenko [44] is based on the addition translation theorem for vector spherical wave functions (VSWFs). In principle, any computational method that solves Maxwell's equations can be employed to calculate the T-matrix, although the computational efficiency, the computer memory requirements, the complexity of the numerical implementation, and the range of practical applicability can be quite variable.

The IIM for the calculation of the T-matrix has drawn scant attention since Johnson's study [40] (with specific applications to relatively small particles) was published in 1988. For example, the IIM is referenced neither in the T-matrix books [20–22] nor in the established T-matrix reference database [38,39]. Moreover, according to the ISI Web of Knowledge, Ref. [40] has previously been cited only 7 times. The use of the IIM in T-matrix calculations can be traced to its application to scattering problems in quantum mechanics [45]. Note that in addition to its application to the solution of Maxwell's equations, the IIM has been applied to the solution of the radiative transfer equation [46]. During the 1990s and early 2000s, significant advancement in relevant numerical techniques and computer resources has been made, and we believe the time has come to revisit the IIM for state-of-the-art numerical implementations.

This study explores the application of a numerical combination of Johnson's IIM method and the SOV (hereafter, IIM+SOV) to light scattering by large nonspherical and inhomogeneous particles. The remainder of the paper is organized as follows: Section 2 outlines the fundamentals of the T-matrix method and the invariant imbedding procedure; Section 3 includes the implementation of the IIM+SOV method to simulate light scattering by representative nonspherical and inhomogeneous particles, and both validates the accuracy and illustrates the efficiency by comparing IIM+SOV method results versus their counterparts computed from other methods; and, Section 4 summarizes our study.

2. Theoretical basis

2.1. The T-matrix

To elaborate the concept of the IIM for the computation of the T-matrix, we begin with the definition of the T-matrix based on the expansion of the incident and scattered fields in terms of VSWFs. The definition of the T-matrix depends on the adopted functional basis. To facilitate a combination of the T-matrix computation and the analytical orientation-average algorithm outlined in Mishchenko et al. [21], we adopt the VSWFs in the exponential form in spherical coordinates. Let us consider the scattering of a plane electromagnetic wave $\overline{\mathbf{E}}^{inc}(\mathbf{r})$ by a finite volume with a non-unity relative refractive index surrounded by an infinite homogeneous, isotropic, and non-absorbing host medium. We expand the incident and scattered fields in terms of VSWFs as:

$$\overline{\mathbf{E}}^{inc}(\mathbf{r}) = \sum_{n=1}^{\infty}\sum_{m=-n}^{n} \overline{\overline{\mathbf{Y}}}_{mn}(\theta,\phi)\overline{\overline{\mathbf{J}}}_{n}(r)\begin{bmatrix} a_{mn} \\ b_{mn} \end{bmatrix}, \tag{1}$$

$$\overline{\mathbf{E}}^{sca}(\mathbf{r}) = \sum_{n=1}^{\infty}\sum_{m=-n}^{n} \overline{\overline{\mathbf{Y}}}_{mn}(\theta,\phi)\overline{\overline{\mathbf{H}}}_{n}(r)\begin{bmatrix} p_{mn} \\ q_{mn} \end{bmatrix}, \quad r > r_{>}, \tag{2}$$

where $r_{>}$ is the radius of the smallest circumscribed sphere of the scattering volume centered at the origin of