Journal of Quantitative Spectroscopy & Radiative Transfer 112 (2011) 1726–1732

Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

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

T-matrix approach to calculating circular polarization of aggregates made of optically active materials

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ARTICLE INFO

Available online 15 February 2011

Keywords:
Aggregate scattering
Circular polarization
Optically active

ABSTRACT

Optical activity is a typical property of the biological materials where left-handed amino-acids and right-handed carbohydrates dominate (so called homochirality). Observationally, optically active materials reveal themselves through the circular polarization in the light they scatter. Thus, circular polarization produced by the optically active particles can serve as a biomarker. It is known that biological (e.g. colonies of bacteria) and pre-biological (e.g. dust in comets) particles often have a complex structure that can be modeled presenting them as aggregates of small monomers. This motivated the development of the *T*-matrix code presented in this paper, which enables calculation of the scattering matrix – including circular polarization – of the light scattered by aggregated optically active particles. The code can be used for modeling the light scattering by biological objects (e.g. colonies of bacteria, blood cells) and for interpretation of the circular polarization produced by the cosmic dust that contains (pre)biological organic, e.g. comet dust or planetary aerosols.

1. Introduction

Many complex organic molecules exist in two forms that are identical except that they pose chirality, i.e., are mirror images of each other. A typical characteristic of life is the homochirality of biological molecules, i.e., predominance of one of the mirror forms of the organic molecules. This characteristic may be manifested on a macroscopic scale through the optical activity of the chiral molecules and, hence, the presence of circular polarization (CP) in the light they scatter. Recently a set of data on circular polarization in comets has been accumulated [1,2]. Characteristics of the cometary CP in the set, specifically an average toward left-handed polarization, could be viewed as evidence of homochiral organics in comet dust similar to that found in meteorites [3]. We have also explored remote sensing capabilities of circular polarization in the laboratory, by studying light scattering from astrobiologically relevant microorganisms and setting these in the context of abiotic minerals [4]. We have found a dependence of the CP on the dichroism of the materials that results in greater circular polarization in absorption bands.

Theoretical and computational tools are needed to confirm whether the presence of chiral organics can produce the observed characteristics of comet circular polarization and explain the results of our laboratory measurements. A well known solution exists for an isolated, optically active sphere [5], yet a single-sphere model for complex comet dust particles or colonies of bacteria is both unrealistic and incapable of explaining recent results.

A significant part of comet dust is in the form of particles having an aggregated structure [6], and such a structure is also plausible for a variety of biological

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0022-4073/$ - see front matter
doi:10.1016/j.jqsrt.2011.02.003

particles. To better account for the non-spherical nature of such particles, we have developed a T-matrix code to predict light scattering and absorption by aggregates of optically active (OA) spheres. We anticipate that this code will be applicable to a variety of astrobiological problems, including the search for materials containing molecules of pre-biological and biological origin in comets, planets, extrasolar planets, and protoplanetary nebulae as well as for studying biological particles in the Earth atmosphere and in the laboratory.

The paper will present the formulation and computational algorithm for calculating the T-matrix for a cluster of OA spheres. As will be shown, the solution can predict the detailed electromagnetic field both within and external to the spheres, and we use this capability in example calculations to demonstrate the veracity of the code. We also present a limited set of calculations that show the effects of OA on circular polarization of aggregated particles.

2. Formulation

The formulation for interactive scattering among a cluster of optically active spheres can be obtained by a merging of the formulations for optically active single spheres and multiple, non-active spheres. We will begin by reviewing the single (or isolated) sphere relations, and then describe the required modifications to the interacting sphere formulation that are needed to account for optical activity.

2.1. The T-matrix for a single OA sphere

The defining characteristic of OA media is that only circularly polarized, homogenous plane waves can propagate in such media without undergoing a change in polarization state. Following the formulation of Bohren and Huffman [7], the electric and magnetic fields propagating within OA media can be constructed from a linear transformation of left and right expansion functions [7], denoted as Q_L and Q_R, i.e.,

$$\begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix} = \mathbf{A} \begin{pmatrix} \mathbf{Q}_L \\ \mathbf{Q}_R \end{pmatrix} \tag{1}$$

in which the matrix $\mathbf{A}$ is

$$\mathbf{A} = \begin{pmatrix} 1 & -\mathrm{i}/\mathrm{m} \\ -\mathrm{im} & 1 \end{pmatrix} \tag{2}$$

The $\mathbf{Q}$ expansion functions satisfy

$$\nabla \times \mathbf{Q}_L = k_L \mathbf{Q}_L \tag{3}$$

$$\nabla \times \mathbf{Q}_R = -k_R \mathbf{Q}_R \tag{4}$$

in which $k_L = 2\pi \mathrm{m}_L/\lambda$ and $k_R = 2\pi \mathrm{m}_R/\lambda$ are the left and right wavenumbers for the medium, with m_L and m_R denoting the relative refractive indices for left and right circularly polarized light. The left and right refractive indices are related to the average (or bulk) refractive index m by

$$\mathrm{m} = \frac{2}{1/\mathrm{m}_L + 1/\mathrm{m}_R} \tag{5}$$

In addition, the left and right refractive indices can be specified by the average m and a complex chiral factor β by

$$\mathrm{m}_L = \frac{\mathrm{m}}{1-\beta \mathrm{m}}, \quad \mathrm{m}_R = \frac{\mathrm{m}}{1+\beta \mathrm{m}} \tag{6}$$

The $\mathbf{Q}$ expansion functions can be represented in the interior of an OA sphere by expansions of the regular vector wave harmonics (VWH) $\mathbf{N}^{(1)}_{mnp}(k\mathbf{r})$, of order n, degree m, and mode p=1 (TM) or 2 (TE). The VWHs satisfy the vector Helmholtz equation

$$\nabla^2 \mathbf{N}^{(1)}_{mnp}(k\mathbf{r}) + k^2 \mathbf{N}^{(1)}_{mnp}(k\mathbf{r}) = 0 \tag{7}$$

as well as

$$\nabla \times \mathbf{N}^{(1)}_{mn1}(k\mathbf{r}) = k\mathbf{N}^{(1)}_{mn2}(k\mathbf{r}), \quad \nabla \times \mathbf{N}^{(1)}_{mn2}(k\mathbf{r}) = k\mathbf{N}^{(1)}_{mn1}(k\mathbf{r}) \tag{8}$$

With this set of basis functions, formulas for the $\mathbf{Q}$ expansion functions will appear as

$$\mathbf{Q}_L(\mathbf{r}) = \sum_{n=1} \sum_{m=-n}^{n} c_{mnL} (\mathbf{N}^{(1)}_{mn1}(k_L\mathbf{r}) + \mathbf{N}^{(1)}_{mn2}(k_L\mathbf{r})) \tag{9}$$

$$\mathbf{Q}_R(\mathbf{r}) = \sum_{n=1} \sum_{m=-n}^{n} c_{mnR} (\mathbf{N}^{(1)}_{mn1}(k_R\mathbf{r}) - \mathbf{N}^{(1)}_{mn2}(k_R\mathbf{r})) \tag{10}$$

in which c_{mnL} and c_{mnR} denote the sought expansion coefficients for the internal field.

Exterior to the sphere, the incident and scattered fields will be represented by the usual expansions of regular and outgoing VWH, i.e.,

$$\mathbf{E}_{inc}(\mathbf{r}) = \sum_{n=1} \sum_{m=-n}^{n} \sum_{p=1}^{2} f_{mnp} \mathbf{N}^{(1)}_{mnp}(k\mathbf{r}) \tag{11}$$

$$\mathbf{E}_{sca}(\mathbf{r}) = \sum_{n=1} \sum_{m=-n}^{n} \sum_{p=1}^{2} a_{mnp} \mathbf{N}^{(3)}_{mnp}(k\mathbf{r}) \tag{12}$$

in which the expansion coefficients f for the incident field will depend on the direction and polarization state of the field. Evaluation of the continuity conditions at the sphere surface will yield a linear relation between the scattering and incident field coefficients, of the form

$$a_{mnp} = \sum_{q=1}^{2} \overline{a}_{n;pq} f_{mnq} \tag{13}$$

in which the coefficients $\overline{a}$ will be a function of the sphere size parameter ka and the left and right refractive indices. These are analogous to the Lorenz–Mie coefficients for non-active spheres. Explicit formulas are

$$\overline{a}_{n;11} = -\frac{V_n(L)A_n(R) + V_n(R)A_n(L)}{D_n} \tag{14}$$

$$\overline{a}_{n;22} = -\frac{W_n(L)B_n(R) + W_n(R)B_n(L)}{D_n} \tag{15}$$

$$\overline{a}_{n;12} = \overline{a}_{n;21} = \frac{W_n(L)A_n(R) + W_n(R)A_n(L)}{D_n} \tag{16}$$

$$D_n = W_n(L)V_n(R) + W_n(R)V_n(L) \tag{17}$$

$$W_n(J) = -(\xi_n(x)\psi'_n(x\mathrm{m}_J)) + \mathrm{m}\psi_n(x\mathrm{m}_J)\xi'_n(x) \tag{18}$$

$$V_n(J) = -(\mathrm{m}\xi_n(x)\psi'_n(x\mathrm{m}_J)) + \psi_n(x\mathrm{m}_J)\xi'_n(x) \tag{19}$$