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A general superposition solution for electromagnetic scattering by multiple spherical domains of optically active media

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ABSTRACT

The superposition solution for scattering by a system of optically active spheres is extended to the case where any of the spheres can be located at points that are either internal and external to the other spheres. The sole restriction on the formulation are that a sphere surface cannot be cut by another surface. The formulation has been integrated into the Multiple Sphere *T* Matrix code, and illustrative calculation results that demonstrate the veracity of the formulation are presented.

1. Introduction

The purpose of this work is to report on an extension to the parameter space available to the Multiple Sphere *T* Matrix (MSTM) code [1] for calculation of the electromagnetic scattering properties of multiple sphere domains. This extension involves a removal of the constraint that limited each sphere to reside fully exterior to all other spheres, i.e., external configurations. Each sphere in the set can now be contained at any point internal or external to any other sphere, with the sole restriction being that the surfaces of different spheres cannot overlap. The various materials making up the system – contained both within and external to the sphere surfaces – can also be optically active.

Comprehensive solutions of Maxwell's time harmonic wave equations have been developed for the separate cases of externally/internally aggregated systems of isotropic (non-active) spheres [2–4] and externally aggregated active spheres [5].[1] These two solutions share many commonalities: they both use superposition to describe the electromagnetic fields in the system, and they both represent the individual components in these superpositions as expansions of vector spherical wave functions (VSWFs). A mathematical welding of these two solutions into a single unit requires nothing more than the same mathematical toolkit used to build the separate pieces, and in this respect the reported formulas are simply bigger and not necessarily better.

On the other hand, the author will submit that this incremental extension of the formulation does make for a "generalized Mie theory" that is about as general as a Mie theory can be. That is, it will identify a mathematical procedure for exactly predicting the electromagnetic field in and about a discretely (i.e., piecewise) inhomogeneous volume of arbitrary configuration, excited by an external field, and subject to the constraint that the boundaries

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[1] An extensive list of references to, and applications of, multiple sphere scattering theory is contained in the comprehensive *T* matrix databases [6,7].

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separating one individual homogeneous element from another are in the form of N_S closed spherical surfaces. Such a system could be an aggregate of N_S homogenous spheres, or it could be a single sphere with N_S (possibly eccentric) layers, or it could be anything in between.

The plan of the paper is to summarily describe the combined internal/external and optically active superposition solution, with emphasis given to the practical implementation of the formulas in the MSTM code. A limit set of example calculation results will be presented, with sole purpose being to demonstrate the validity of the code.

2. Formulation

2.1. Physical configuration

The system consists of N_S spherical surfaces, with each characterized by a dimensionless size parameter $x^i = ka^i = 2\pi a^i/\lambda$, where a^i is the sphere radius and λ the wavelength in vacuum, a left–right pair of complex refractive indices $\mathbf{m}^i = (\mathrm{m}_L^i,\ \mathrm{m}_R^i)$ for the medium contacting the *inside* surface of the sphere, and a dimensionless position vector $k\mathbf{r}^i = k(X^i, Y^i, Z^i)$, relative to a common target origin, that denotes the origin of the spherical surface, for $i = 1, 2, \ldots N_S$. There is no restriction placed on the location of the sphere origins, with the sole exception that the surfaces of any two spheres cannot overlap. In other words, there can only be one value of $\mathbf{m}^i$ for each surface i.

Each spherical surface i will have an associated *host sphere* $h(i)$, that being the sphere whose refractive index $\mathbf{m}^h$ is in contact with the exterior surface of i. In this convention the external medium (that which extends to infinity) is associated with an imaginary sphere denoted as 0, with the medium refractive index denoted $\mathbf{m}^0$. This convention is illustrated in Fig. 1, for which spheres 1, 2, and 3 have host 0, spheres 4, 5, and 6 have host 3, and sphere 7 has host 6. There is no limitation to the ordering of the spheres – spheres can contain spheres containing spheres, and so on.

A spherical surface, say surface i, will also have associated with it subsets of N_S corresponding to the *external* and *internal* neighboring spherical surfaces. The exterior neighbor set for i, denoted as $\mathcal{N}^i_{ext}$, is all surfaces j that have $h(j) = h(i)$, i.e., the same host as i. The interior set for i, denoted as $\mathcal{N}^i_{int}$, contains all surfaces j that have $h(j) = i$, and the number of elements in this interior set will be denoted as N_S^i. Referring to Fig. 1, surface 3 has $\mathcal{N}^3_{ext} = (1,2)$ and $\mathcal{N}^3_{int} = (4,5,6)$. The set $\mathcal{N}^0_{int}$ will include all the external spheres, i.e., the spheres in contact with the external medium. A general rule is that $\mathcal{N}^i_{ext}$ will include all members of $\mathcal{N}^{h(i)}_{int}$ except i. The definition of these sets will help simplify the subsequent formulation.

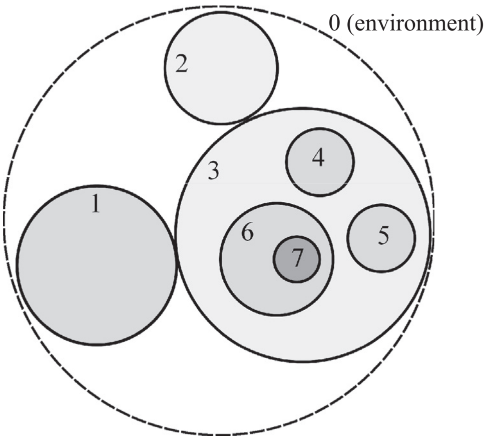

Fig. 1. Internal and external spheres.

2.2. Optically active formulation

In what follows the electric **E** and magnetic **H** complex amplitude vectors will be assumed dimensionless, with magnitudes scaled by those corresponding to the incident fields (i.e., the fields in the absence of the particle). In optically active media, Maxwell's equations for time harmonic fields (of factor $\exp(-\mathrm{i}\omega t)$) appear as [8]

$$\nabla \times \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix} = \frac{k}{1-\beta^2\mathrm{m}^2}\begin{pmatrix} \beta\mathrm{m}^2 & \mathrm{i} \\ -\mathrm{i}\mathrm{m}^2 & \beta\mathrm{m}^2 \end{pmatrix}\cdot\begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix} \tag{1}$$

where $\mathrm{m} = \sqrt{\epsilon/\epsilon_0}$ is the bulk refractive index of the medium and β is the dimensionless chirality factor. A linear transformation of the electric and magnetic fields, of the form

$$\begin{pmatrix} \mathbf{E} \\ (\mathrm{i}/\mathrm{m})\mathbf{H} \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} \mathbf{Q}_L \\ \mathbf{Q}_R \end{pmatrix} \tag{2}$$

will diagonalize Eq. (1), so that

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

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

where the left and right wavenumbers are given by

$$k_L = \mathrm{m}_L k = \frac{\mathrm{m}k}{1-\beta\mathrm{m}} \tag{5}$$

$$k_R = \mathrm{m}_R k = \frac{\mathrm{m}k}{1+\beta\mathrm{m}} \tag{6}$$

2.3. VSWF representation and continuity relations for spherical boundaries

Eqs. (3) and (4) provide a means of representing the left and right field vectors $\mathbf{Q}_L$ and $\mathbf{Q}_R$ as expansions of vector spherical wave functions (VSWFs). The VSWFs, of degree m, order n, mode p ($=1,2$ for TE, TM), and type ν ($=1$, 3 for regular and outgoing) satisfy

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

$$\nabla \times \mathbf{N}^{(\nu)}_{mnp}(k\mathbf{r}) = k\mathbf{N}^{(\nu)}_{mn3-p}(k\mathbf{r}) \tag{8}$$

Note that the convention $3-p$ in Eq. (8) switches from one mode to the other.