LIGHT SCATTERING BY AXISYMMETRIC PARTICLES: A NEW APPROACH WITH THE SPECIAL CHOICE OF SCALAR POTENTIALS

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ABSTRACT

A new approach to solve the problem of light scattering by particles with an axial symmetry is developed. The electromagnetic fields are divided in two (axisymmetric and non-axisymmetric) parts. The scattering problem formulated in the integral form is solved separately for each of the parts using specially chosen scalar potentials. The potentials are expanded in terms of the spherical wave functions, and the expansion coefficients are determined from solution of the infinite systems of linear algebraic equations. A numerical code based on the approach is created and tested for spheroids, finite size cylinders, and Chebyshev particles.

1. INTRODUCTION

There are many methods to calculate the light scattering by non-spherical particles (see, e.g., Mishchenko et al., 2000 and references therein). Some of the methods are universal and can be applied to scatterers of any shape. However, in applications one mostly considers axisymmetric particles – spheroids, finite-sized circular cylinders, etc. – otherwise the calculations become too computational time-consuming.

The light scattering problem for spheroids (the simplest form of axisymmetric particles besides spheres) is of particular interest. In this case the boundary of the scatterer coincides with a coordinate surface of the spheroidal system, and one can separate variables in the scalar Helmholtz equation. Several solutions utilizing this approach (e.g., Asano and Yamamoto, 1975; Farafonov, 1983) differ mainly in the choice of the scalar potentials.

Asano and Yamamoto (1975) used the Debye potentials which are applied in the Mie theory for spheres. Quite different potentials were chosen by Farafonov (1983). He divided the electromagnetic fields in two parts: an axisymmetric part without a dependence on the azimuthal angle and a non-axisymmetric part whose averaging over this angle gave zero. Then the Abraham potentials connected with the azimuthal components of the electromagnetic fields were selected to describe the field components independent of the azimuthal angle. For the components that depend on this angle, a superposition of the Debye potentials and the vertical components of the Hertz vector (used in the solution of the light scattering problem for infinitely long cylinders) were applied.

A comparison of numerical results obtained within the approaches of Asano and Yamamoto and of Farafonov has shown that the latter is more efficient especially for very elongated or fattened particles (Voshchinnikov and Farafonov, 1983; Voshchinnikov, 1996). For example, the number of terms in the sums for cross-sections necessary to reach a given accuracy depends on the parameter $2\pi a/\lambda$ (a is the major semiaxis of the spheroid, λ the wavelength of incident radiation) and does not depend on the shape of particles. In the solution of Asano and Yamamoto, this number and consequently the computational time essentially grow with an increase of the aspect ratio a/b, which demonstrates an important role of the proper choice of the potentials.

We suggest a new method to compute the optical properties of axisymmetric particles that should combine the advantages of the approach of Farafonov and the high capacity of the T-matrix method. The scattering problem is divided in two (axisymmetric and non-axisymmetric) parts and the scalar potentials for each of the parts are nearly similar to those used for spheroids. The potentials are expanded in terms of the spherical wave functions, and the problem is formulated in the form of integral equations.

In previous works (Farafonov et al., 1999; Farafonov, 2000) we described the main idea of the method, gave some formulae for the TM mode and made test calculations in the case of an axial incidence of radiation on spheroids. In this paper we consider the more complex case of the TE mode, and present computational results for oblique incidence (for both TE and TM modes) concentrating on finite cylinders and Chebyshev particles.

2. BASIC EQUATIONS

Let us consider the light scattering by a single particle with an axial symmetry and introduce the Cartesian system (x, y, z) with the axis z along the symmetry axis of the particle. In the spherical polar coordinates (r, θ, φ) the surface of the particle S is defined by the equation $r = r(\theta)$.

A plane electromagnetic wave propagating at the incident angle α to the particle symmetry axis (the z axis) can be represented as a superposition of the waves of two types: the TE and TM modes. The incident, scattered and internal electromagnetic fields are denoted by $\vec{E}^{(j)}$ and $\vec{H}^{(j)}$ with $j = 0, 1$ and 2, respectively; μ_j is the magnetic permeability, and ε_j the complex permittivity outside ($j = 1$) and inside ($j = 2$) the particle. The wavenumbers in the media are $k_j = \sqrt{\varepsilon_j \mu_j}\, k_0$, where $j = 1, 2$; $k_0 = 2\pi/\lambda$ is the wavenumber in vacuum, λ the wavelength.

The incident, scattered, and internal fields are represented as the sums

$$\vec{E}^{(j)} = \vec{E}_1^{(j)} + \vec{E}_2^{(j)}, \quad \vec{H}^{(j)} = \vec{H}_1^{(j)} + \vec{H}_2^{(j)}, \quad j = 0, 1, 2, \tag{1}$$

where $\vec{E}_1^{(j)}$ and $\vec{H}_1^{(j)}$ do not depend on the azimuthal angle φ, and averaging of $\vec{E}_2^{(j)}$ and $\vec{H}_2^{(j)}$ over all values of this angle gives zero. The scattering problem is solved separately for the axisymmetric and non-axisymmetric components of the fields. Such a separation is possible because of the commutation of the operator corresponding to the diffraction problem and the operator $L_z = \partial/\partial\varphi$ (see Farafonov 2000 for more details).

2.1. Solution of the axisymmetric problem

We introduce the scalar potentials

$$p^{(j)} = E_{1\varphi}^{(j)} \cos\varphi, \quad q^{(j)} = H_{1\varphi}^{(j)} \cos\varphi, \tag{2}$$

where $E_{1\varphi}^{(j)}$ and $H_{1\varphi}^{(j)}$ are the azimuthal components of $\vec{E}_1^{(j)}$ and $\vec{H}_1^{(j)}$. Other components of the fields can be expressed via the azimuthal components using Maxwell's equations. Easy to see that the potentials satisfy the scalar Helmholtz equation

$$\Delta p^{(j)} + k_j^2 p^{(j)} = 0, \quad \Delta q^{(j)} + k_j^2 q^{(j)} = 0. \tag{3}$$

Note that the problem can be solved for the potentials p (the TE mode) and q (the TM mode) separately.

Thus, the scattering problem is reduced to a solution of the scalar equation (**??**) with the boundary conditions and the conditions at infinity (Farafonov et al., 1999). Now we reformulate the scattering problem in terms of integral equations. One can get the following integral equation for the scalar potential $p^{(2)}$ valid inside the particle, i.e. $\vec{r} \in \mathcal{D}$ (see Farafonov, 2000 for details):

$$\int_S \left\{ p^{(2)}(\vec{r}\,') \, \frac{\partial G(\vec{r}, \vec{r}\,')}{\partial n} - \left[\frac{\mu_1}{\mu_2} \frac{\partial p^{(2)}(\vec{r}\,')}{\partial n} + \left(\frac{\mu_1}{\mu_2} -1 \right) \frac{1}{\sqrt{(r')^2 + \left[(r')'_{\theta'}\right]^2}} \left(1 - \frac{(r')'_{\theta'}}{r\,'} \cot\theta' \right) \times p^{(2)}(\vec{r}\,') \right] G(\vec{r}, \vec{r}\,') \right\} \mathrm{d}S' = -p^{(0)}(\vec{r}) \,. \tag{4}$$

The same equation with the only change of $-p^{(0)}$ by $p^{(1)}$ can be obtained for the region $\vec{r} \in R^3 \setminus \bar{\mathcal{D}}$.

The corresponding equations for the potentials $q^{(j)}$ are similar to given ones after the replacement of $p^{(j)}$ by $q^{(j)}$ and μ_j by ε_j (see Farafonov et al., 1999).

The scalar potentials are expanded in terms of the spherical wave functions

$$p^{(0)} = \sum_{l=1}^{\infty} a_l^{(0)} \; j_l(k_1 r) \, P_l^1(\cos\theta) \, \cos\varphi, \tag{5}$$

where $j_l(k_1 r)$ is the spherical Bessel function, $P_l^m(\cos\theta)$ the associated Legendre function. Easy to get the expansion coefficients of $p^{(0)}$. In the expansions of $p^{(1)}$ and $p^{(2)}$ instead of $j_l(k_1 r)$ one should use the Hankel function of the first kind $h_l^{(1)}(k_1 r)$ and $j_l(k_2 r)$, respectively.

We substitute the expansions of the potentials and of the diadic Green function into the integral equations. From the orthogonality of the wave functions over a spherical surface that is totally inside the scatterer, one can derive systems of linear algebraic equations, for instance the following one from Eq. (**??**):

$$\sum_{n=1}^{\infty} \alpha_{ln}^{(2)} \, a_n^{(2)} = -a_l^{(0)}, \quad l = 1, 2, \dots \,, \tag{6}$$

where the matrix elements $\alpha_{ln}^{(2)}$ are the surface integrals of products of the spherical wave functions and their derivatives. Likewise one can get the system for coefficients $a_n^{(1)}$ and $a_n^{(2)}$ from the second integral equation including the potentials $p^{(1)}$ and $p^{(2)}$. In this system the matrix elements $\alpha_{ln}^{(1)}$ coincide with $\alpha_{ln}^{(2)}$ after the replacement of $j_l(k_1 r)$ by $h_l^{(1)}(k_1 r)$.

For the potentials $q^{(j)}$, the problem is solved in a similar way – all equations become the same after the changes $p^{(j)} \to q^{(j)}$, $\mu_j \to \varepsilon_j$ and $a_n^{(j)} \to b_n^{(j)}$ (see Farafonov et al., 1999).

2.2. Solution of the non-axisymmetric problem

To determine the non-axisymmetric components of the electromagnetic fields $\vec{E}_2^{(j)}$ and $\vec{H}_2^{(j)}$, we utilize the scalar potentials $U^{(j)}$ and $V^{(j)}$. The former is the z-component of the Hertz vector and the latter the Debye potential. For the TE mode, one has

$$\begin{aligned}
\vec{E}_2^{(j)} &= \vec{\nabla} \times \left(U^{(j)}\, \vec{i}_z + V^{(j)}\, \vec{r} \right), \\
\vec{H}_2^{(j)} &= \tfrac{1}{i\mu_j k_0} \vec{\nabla} \times \vec{\nabla} \times \left(U^{(j)}\, \vec{i}_z + V^{(j)}\, \vec{r} \right);
\end{aligned} \tag{7}$$

the corresponding equations for the TM mode were given in Farafonov et al. (1999).

The boundary conditions can be formulated in terms of the potentials $U^{(j)}$ and $V^{(j)}$ as well. They are essentially simplified in the standard case of non-magnetic media ($\mu_1 = \mu_2 = 1$).

The integral equations for the potentials $U^{(j)}$ and $V^{(j)}$ are derived like the equations for the potentials $p^{(j)}$ (e.g., Eq. (**??**)). For instance, the equation for $U^{(2)}$ is

$$\begin{aligned}
\int_S \Bigg\{ & U^{(2)}(\vec{r}\,') \frac{\partial G(\vec{r},\vec{r}\,')}{\partial n} - \Bigg[\frac{\partial U^{(2)}(\vec{r}\,')}{\partial n} + \left(\frac{\varepsilon_1}{\varepsilon_2} - 1 \right) \\
& \times \frac{(r')'_{\theta'}}{\sin\theta' r' \sqrt{(r')^2 + \left[(r')'_{\theta'}\right]^2}} \Bigg(r' \cos\theta' \frac{\partial U^{(2)}}{\partial r'}(\vec{r}\,') \\
& - \sin\theta' \frac{\partial U^{(2)}(\vec{r}\,')}{\partial \theta'} + (r')^2 \frac{\partial V^{(2)}(\vec{r}\,')}{\partial r'} + r' \\
& \times V^{(2)}(\vec{r}\,') \Bigg) \Bigg] G(\vec{r},\vec{r}\,') \Bigg\} \mathrm{d}S' = -U^{(0)}(\vec{r}), \quad \vec{r} \in \mathcal{D}.
\end{aligned} \tag{8}$$

The expansions of $U^{(j)}$ and $V^{(j)}$ and of the diadic Green function in terms of the spherical wave functions are substituted in the integral equations.

Now, in the same way as we got the system (**??**) for the coefficients $a_n^{(2)}$, one can obtain the infinite systems of linear algebraic equations for the expansion coefficients $a_{mn}^{(2)}$ and $b_{mn}^{(2)}$ of the potentials $U^{(j)}$ and $V^{(j)}$

$$\begin{aligned}
\sum_{n=m}^{\infty} \left(\alpha_{1,mln}^{(2)}\, k_1 a_{mn}^{(2)} + \beta_{1,mln}^{(2)}\, b_{mn}^{(2)} \right) &= -k_1 a_{ml}^{(0)}, \\
\sum_{n=m}^{\infty} \left(\alpha_{2,mln}^{(2)}\, k_1 a_{mn}^{(2)} + \beta_{2,mln}^{(2)}\, b_{mn}^{(2)} \right) &= -b_{ml}^{(0)},
\end{aligned} \tag{9}$$

where $m = 1, 2, ...; l = m, m+1, ...$ and the matrix elements $\alpha_{1,mln}^{(2)}$, $\alpha_{2,mln}^{(2)}$, $\beta_{1,mln}^{(2)}$, and $\beta_{2,mln}^{(2)}$ are the surface integrals of products of the spherical wave functions and their derivatives. The systems for $a_{mn}^{(1)}$ and $b_{mn}^{(1)}$ appear analogically.

With known coefficients of the potential expansions, it is easy to find the extinction and scattering cross-sections and other characteristics of the scattered radiation.

3. NUMERICAL TESTS

We have created a computer code that realizes our approach. The code was tested by comparison with results obtained using available codes basing on the Separation of variables method for spheres and spheroids of various sizes, compositions, and aspect ratios.

3.1. Finite cylinders

Finite size cylinders (and spheroids) belong to the class of “weakly non-convex” particles for which the scattering problem in the given form should be unambiguously solvable according to theoretical works (see Kyurkchan, 1994 and references therein).

As illustration we have calculated and compared in Figs. 1–2 the scattering cross-sections of finite cylinders and spheroids of same volumes and aspect ratios. Note the effects of the sharp edges of the cylinders.

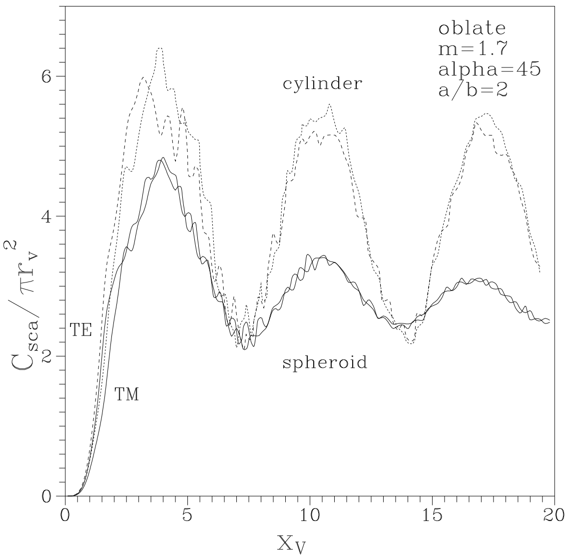

Figure 1: The scattering cross-section divided by the shadow area of the equivolume sphere for oblate spheroids (solid lines) and finite size cylinders of the same volume (dashed lines). The ratio of diameter to length of the cylinders is equal to the semiaxis ratio of spheroids (a/b). The angle of incidence of radiation (TE and TM modes) $\alpha = 45°$; refractive index m =1.7.

We have also compared our code with the standard T-matrix program of Barber and Hill (1990) for finite cylinders and spheroids and found that our program was nearly as fast as their code (in double procession).

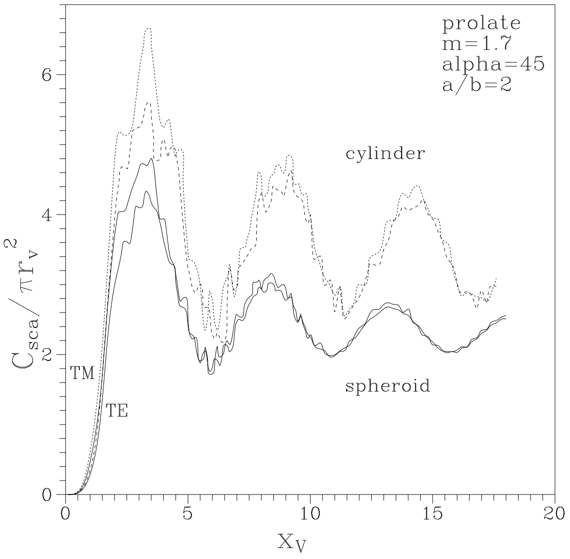

Figure 2: The same as in Fig. 1 but for prolate particles.

3.2. Chebyshev particles

In contrast to the scatterers considered in the previous subsection, the Chebyshev particles having the surface equation $r(\theta) = r_0[1 + \varepsilon \cos(n\theta)]$ can be concave (if $|\varepsilon| < (n^2 + 1)^{-1}$). In this case our solution can be explicitly proved if the analytic continuations of the scattered and internal fields have a non-empty common region including of a ring with the center at the coordinate system origin. This condition can be formulated as

$$\sigma_1(r_0, n, \varepsilon) < \sigma_2(r_0, n, \varepsilon) \qquad (10)$$

where σ_1 and σ_2 are the distances of peculiar points from the coordinate system origin for the scattered and internal fields, respectively. An investigation of such conditions in the scalar case has been done by Kyurkchan (1994).

As an example we give in Table 1 some results for the Chebyshev particles with n = 10 and three values of ε = 0.01, 0.05, and 0.07. In the first and second cases the particles are Rayleigh and non-Rayleigh ones, respectively. Both particles are weakly non-convex, but the difference is well seen. In the third case the condition of weakly non-convexity (Eq. (**??**)) is not valid (for n =10, $\sigma_1 = \sigma_2$ at $\varepsilon \approx$ 0.663), and our solution works unsatisfactorily in accordance with the theoretical predictions. A similar situation occurs for other values of the parameters α and m.

Table 1: Normalized scattering cross-sections $C_{\rm sca}/\pi r_V^2$ for the Chebyshev particles with n =10 and different values of r_0 and ε. In the numbers, the digits are given only when they coincide in $C_{\rm sca}$ and $C_{\rm ext}$ (refractive index m =1.5).

	ε		
r_0	0.01	0.05	0.07
1.0	0.2151960	0.2185379	0.222249
2.0	1.797344	1.7905	1.785
3.0	3.416862	3.421	3.4
3.5	4.074654	4.073	4.1
4.0	4.0476801	4.067	
5.0	3.96219	4.16	
6.0	2.90559	2.96	
7.0	1.8566	1.93	

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