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SOLUTIONS OF THE ELECTROSTATIC PROBLEM FOR HIGHLY ECCENTRIC PARTICLES WITH AXIAL SYMMETRY

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ABSTRACT. The problem of interaction between the electrostatic field and an axisymmetric particle with analytical shape in the spheroidal coordinates is considered. The proposed solutions are based on two of the light scattering methods having different numerical properties, namely the separation of variables and extended boundary condition methods. The relation between the electrostatic fields and electromagnetic radiation in the far-field zone is revealed.

1. Introduction

The electrostatic model of a particle in the uniform electric field is often used for the approximation of scattering by small particles in various fields of applications including nano-scale optics [1, 2].

The distortion of the uniform field by particles with canonical shapes (spheres, ellipsoids) has been found analytically in the classical monograph [3]. The electrostatic problem has also been solved for confocal and non-confocal multilayered ellipsoids [4, 5], clusters of spheres [6, 7], and spheres near a plane [8]. Besides these geometries generally-shaped axisymmetric particles are widely applied. However only numerically intensive methods, e.g. the finite elements methods or the discrete dipole approximation, are available for modelling them.

In the electromagnetic theory such methods as generalised separation of variables (gSVM) and extended boundary conditions (EBCM) methods were shown to be highly efficient for such shapes [9]. Despite having similar formulation these methods posses different numerical properties.

In this paper we use the gSVM and EBCM methods to solve the electrostatic problem for axisymmetric particles with analytical shapes. We extend our previous work [10] by providing solutions in the spheroidal coordinate system, that allows obtaining numerically stable results for highly oblate and prolate particles.

2. Formulation of the problem

Let us consider a particle in the uniform electric field $\vec{E}^{\mathrm{inc}}$. The particle axisymmetric surface in the spheroidal coordinates (ξ, η, φ) is defined by a single-valued function

$$\xi = \xi(\eta).$$

The electric fields inside and outside the particle are derivable from the scalar potentials

$$\vec{E} = \nabla\Phi$$

that satisfy the Laplace equation

$$\Delta\Phi = 0. \tag{1}$$

At the particle surface S the potentials are related with the boundary conditions postulating the continuity of the tangential components of the electric field densities and the normal components of the electric induction vectors $\vec{B} = \varepsilon\vec{E}$

$$\left.\begin{aligned} \Phi^{\mathrm{inc}} + \Phi^{\mathrm{sca}} &= \Phi^{\mathrm{int}}, \\ \varepsilon_1 \frac{\partial\left(\Phi^{\mathrm{inc}} + \Phi^{\mathrm{sca}}\right)}{\partial n} &= \varepsilon_2 \frac{\partial\Phi^{\mathrm{int}}}{\partial n} \end{aligned}\right\}_{\xi\in S}, \tag{2}$$

where Φ^{inc} and Φ^{sca} are the incident and perturbed parts of the external field potential, Φ^{int} is the internal potential, ε_1 and ε_2 are the complex dielectric permittivities of the media outside and inside of the particle respectively.

3. Solution of the problem

3.1. Expansion of the scalar potentials. The known solutions of the Laplace equation (1) in the prolate spheroidal coordinate system are

$$\psi^1_{ml}(\xi,\eta) = P^m_l(\xi)\bar{P}^m_l(\eta)\cos(m\varphi), \tag{3}$$

$$\psi^2_{ml}(\xi,\eta) = Q^m_l(\xi)\bar{P}^m_l(\eta)\cos(m\varphi), \tag{4}$$

where $l \geq m \geq 0$, $P^m_l(\xi)$ and $Q^m_l(\xi)$ are the associated Legendre functions of the first and second kinds, $\bar{P}^m_l(\eta) = \sqrt{\frac{(2l+1)}{2}\frac{(l-m)!}{(l+m)!}}P^m_l(\eta)$. In the oblate spheroidal coordinates one should use radial functions $P^m_l(i\xi)$, $Q^m_l(i\xi)$.

The scalar potentials Φ in the spheroidal coordinate system can be expanded in infinite series of the functions (3) or (4)

$$\begin{matrix}\Phi^{\mathrm{inc}} \\ \Phi^{\mathrm{int}}\end{matrix} = \sum_{m=0}^{\infty}\sum_{l=m}^{\infty} \begin{matrix}b^{\mathrm{inc}}_{ml} \\ b^{\mathrm{int}}_{ml}\end{matrix} \left(\frac{d}{2}\right)^{l} \psi^1_{ml}, \qquad \Phi^{\mathrm{sca}} = \sum_{m=0}^{\infty}\sum_{l=m}^{\infty} b^{\mathrm{sca}}_{ml}\left(\frac{d}{2}\right)^{-l-1}\psi^2_{ml}. \tag{5}$$

Here d is the focal distance of the coordinate system.

3.2. Applied field potential expansion coefficients. For each component of the applied field represented in the corresponding Cartesian coordinates as

$$\vec{E}^{\mathrm{inc}} = \vec{E}^{\mathrm{inc}}_x + \vec{E}^{\mathrm{inc}}_y + \vec{E}^{\mathrm{inc}}_z$$

the electrostatic problem can be solved independently. As the z-component of the field

$$\vec{E}^{\mathrm{inc}}_z = E^{\mathrm{inc}}_z \vec{i}_z = E^{\mathrm{inc}}_z \frac{d}{2}\xi\eta,$$

its only non-zero expansion coefficient is

$$b_{01}^{\mathrm{inc},z} = E_z^{\mathrm{inc}} \sqrt{\frac{2}{3}}.$$

In the same manner for the x-component we obtain the only non-zero expansion coefficient $b_{11}^{\mathrm{inc},x}$. Because of the symmetry of the problem the solution for the $\vec{E}_y^{\mathrm{inc}}$ is similar to that for the $\vec{E}_x^{\mathrm{inc}}$. Hence, one should solve the problem only for the cases $m = 0$ and $m = 1$.

3.3. Generalised separation of variables method. In the generalised separation of variables method one substitutes the potentials expansions (5) in the boundary conditions (2), then multiplies the first equation by $\bar{P}_n^m(\eta)$ and the second by $h_\varphi \sqrt{h_\eta^2 + {\xi'_\eta}^2 h_\xi^2}\, \bar{P}_n^m(\eta)$ and integrates each of them over η. Here h_ξ, h_η, h_φ are the scale factors. This yields infinite systems of linear equations relative the unknown expansion coefficients

$$\begin{pmatrix} A_1 & -A_2 \\ \varepsilon B_1 & -B_2 \end{pmatrix} \begin{pmatrix} \vec{b}^{\mathrm{int}} \\ \vec{b}^{\mathrm{sca}} \end{pmatrix} = - \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} \vec{b}^{\mathrm{inc}},$$

where A_i, B_i are infinite matrices, $\varepsilon = \varepsilon_2/\varepsilon_1$.

3.4. Extended boundary conditions method. The boundary conditions (2) can be formulated in the integral form

$$\int_S \left\{ \Phi^{\mathrm{int}}(\vec{r}') \frac{\partial G(\vec{r},\vec{r}')}{\partial n} - \varepsilon \frac{\partial \Phi^{\mathrm{int}}(\vec{r}')}{\partial n} G(\vec{r},\vec{r}') \right\} ds' = \begin{cases} -\Phi^{\mathrm{inc}}(\vec{r}), & \vec{r} \in \Gamma, \\ \Phi^{\mathrm{sca}}(\vec{r}), & \vec{r} \in R^3 \backslash \Gamma, \end{cases} \tag{6}$$

where $G(\vec{r},\vec{r}') = 1/|\vec{r} - \vec{r}'|$ is the free-space scalar Green's function. By substituting the potentials expansions (5) and the Green's function expansion [29] in these boundary conditions one obtains infinite system of linear equations

$$B^S \vec{b}^{\mathrm{int}} = -\vec{b}^{\mathrm{inc}}, \qquad B^R \vec{b}^{\mathrm{int}} = \vec{b}^{\mathrm{sca}}.$$

Usually one first solves the first part for the unknown expansion coefficients b_{ml}^{int} and then finds the coefficients b_{ml}^{sca} by using the second part of the relation.

3.5. Far-field optical characteristics. The electrostatic fields obtained above can be used to approximate the near-fields of the electromagnetic scattering by a small particle excited with a plane wave.

If $\vec{E}^{\mathrm{inc}}$ is aligned along the z-axis the asymptotic form of the scattered potential

$$\Phi^{\mathrm{sca}} \sim b_{01}^{\mathrm{sca}} \frac{\cos\theta}{r^2} \sqrt{\frac{1}{6}} \quad (r \longrightarrow \infty),$$

that can be recognized as a potential of a dipole with polarizability $\alpha_z = \frac{1}{3} b_{01}^{\mathrm{sca}}/b_{01}^{\mathrm{inc}}$. Similar analysis holds for the other orientations of the $\vec{E}^{\mathrm{inc}}$. Then the scattering matrix elements and the optical cross-sections can be found from the well-known relations [3].

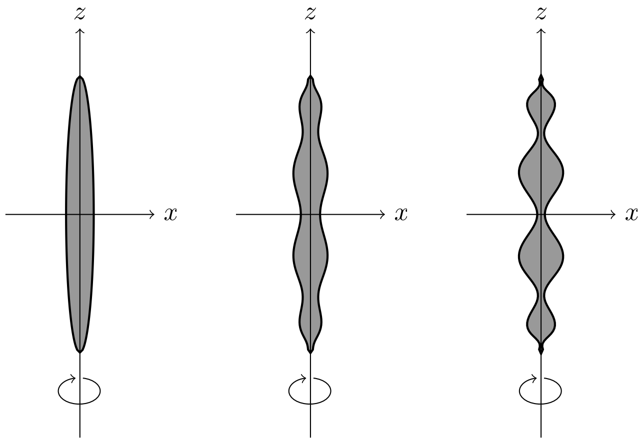

Figure 1. Sample particles for which accurate numerical results were obtained with the proposed methods: a prolate spheroid with $a/b = 10$ and spheroidal Chebyshev particles with the waviness parameter $N = 10$, deformation parameters $\varepsilon = 0,03$ and $\varepsilon = 0,07$.

4. Numerical Results

Comparison of cross-sections obtained for the sample particles (see fig. 1) with the presented methods (gSVM, EBCM) and the DDA has confirmed that electrostatic approximation provides more than 95% accuracy for scatterers with the size parameter $x_V = 2\pi r_V/\lambda < 0.1$. At the same time the aspect raito may be quite large (e.g., $a/b = 20$) and hence the particle length may of the same order of magnitude as the wavelength. Here λ is the wavelength of the incident radiation, r_V is the radius of the equivolume sphere.

The gSVM and EBCM methods in the electrostatic limit were implemented within the ScattPy python package [11] and are available for public use. For more details see http://scattpy.github.com.

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