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Analytical long-wavelength approximation for parallelepipeds

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ABSTRACT

We suggest a new analytical long-wavelength approximation for rectangular parallelepipeds based on replacement of the internal field with a uniform one. The approximation is not quite accurate (the typical accuracy is of the order of about 10%) but is extremely simple and works in a sufficiently wide region of parameter values.

1. Introduction

The most known long-wavelength approximation in the light-scattering theory is the approximation used by Lord Rayleigh to derive simple expressions for the optical properties of ellipsoids small in comparison with the wavelength of the incident plane wave [1]. The approximation has been naturally extended to layered ellipsoids (see, e.g., [2,3]) and ensembles of spheres [4,5]. Recent improvements of the approximation for homogeneous ellipsoids are briefly discussed, e.g., in [6]. Note that the expressions are completely analytical only in the case of spheroids.

For small non-ellipsoidal scatterers, to find their optical properties within the Rayleigh approximation, one needs to numerically solve the corresponding electrostatic problem [7]. It can be done by different methods (see, e.g., their discussion in [8]). Numerical results have been obtained for a number of shapes: finite cylinders, cones, semispheres, etc. (see, e.g., [9,10] and references therein). In particular, dielectric rectangular parallelepipeds have been considered in some detail in [11]. Though the well developed iterative method suggested in [8] to treat small arbitrary shaped scatterers is called analytical, it involves multiple integrals, which is not much simpler than usual numerical solution of integral equations.

An approximate approach to the Rayleigh approximation for any axisymmetric particles has been presented in [12]. It is shown that assuming that the internal field is uniform, one can express polarizability through a one-dimensional integral that can be found analytically for many different shapes.

In this paper we apply an analog of the extended boundary condition method (EBCM – see [13,14] and references therein) to solve the three-dimensional electrostatic problem for a nearly arbitrary shaped particle, which gives the ground for understanding of the nature of the uniform internal field approximation and its comparison with the Rayleigh approximation. Note that such a simplification of the EBCM may be also useful for consideration of not yet quite clear properties of this method [15].

Applying the uniform internal field approximation, we obtain a simple analytical expression for polarizability of rectangular parallelepipeds. Applicability and accuracy of this expression are discussed, and a comparison with the Rayleigh approximation for ellipsoids is made. Note that

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an interest to long-wavelength approximations weakened when powerful computers appeared, but it has to some extend increased recently due to popularity of nano-technologies (see, e.g., [16]).

2. Solution of three-dimensional electrostatic problem by EBCM analog

Let us consider a three-dimensional particle placed in the uniform electric field $\vec{E}_0$. We introduce Cartesian coordinates whose origin is inside the particle (and coincides with the center of the particle when it exists) and the spherical coordinates (r, θ, φ) in such a way that

$$x = r \sin\theta \cos\varphi, \quad y = r \sin\theta \sin\varphi, \quad z = r\cos\theta. \tag{1}$$

We confine our consideration by star-like particles, i.e. by particles whose surface equation can be written in the form $r = r(\theta, \varphi)$.

To solve the electrostatic problem, we use the standard scalar potentials $\Phi(\vec{r})$, related to the electric fields $\vec{E}(\vec{r})$ as follows [17]:

$$\vec{E} = -\nabla\Phi. \tag{2}$$

The potential of the external field is denoted by $\Phi_1^{(1)}$, the potential of the field arisen due to the particle presence by $\Phi_2^{(1)}$, and the potential of the internal field by $\Phi_1^{(2)}$. Note that the potentials with the lower index 1 and 2 are regular and irregular at the coordinate origin, respectively. The upper indices 1 and 2 correspond to the fields outside and inside the particle, respectively. From physical reasons $\Phi_2^{(2)} = 0$.

From the Maxwell equations we find that all the potentials satisfy the Laplace equation:

$$\Delta\Phi = 0. \tag{3}$$

The boundary conditions at the particle surface can be expressed using the potentials as follows:

$$\left.\begin{aligned} &\Phi_1^{(1)} + \Phi_2^{(1)} = \Phi_1^{(2)}, \\ &\frac{\partial(\Phi_1^{(1)} + \Phi_2^{(1)})}{\partial n} = \varepsilon \frac{\partial \Phi_1^{(2)}}{\partial n} \end{aligned}\right\}_{\vec{r} \in S}, \tag{4}$$

where $\partial/\partial n$ is the derivative along the outward normal to the particle surface S, ε the ratio of the dielectric permittivity of the particle to that of the surrounding medium.

The Laplace Equation (3) written in spherical coordinates has the following solutions that can be found by using the separation of variables:

$$\Psi_{ml}^{(1)}\left(\vec{r}\right) = r^l \psi_{ml}(\theta,\varphi), \quad \Psi_{ml}^{(3)}\left(\vec{r}\right) = \frac{1}{2l+1} r^{-(l+1)} \psi_{ml}(\theta,\varphi), \tag{5}$$

where the angular functions $\psi_{ml}(\theta, \varphi)$ can be of two kinds:

$$\begin{aligned} \psi_{mle}(\theta,\varphi) &= \frac{2-\delta_{0m}}{2\pi} \overline{P}_l^m(\cos\theta)\cos m\varphi, \\ \psi_{mlo}(\theta,\varphi) &= \frac{2-\delta_{0m}}{2\pi} \overline{P}_l^m(\cos\theta)\sin m\varphi. \end{aligned} \tag{6}$$

Here

$$\overline{P}_l^m(\cos\theta) = \sqrt{\frac{(2l+1)}{2}\frac{(l-m)!}{(l+m)!}}\, P_l^m(\cos\theta), \tag{7}$$

where $P_l^m(\cos\theta)$ are the associated Legendre functions of the first kind, $\delta_{0m} = 1$ for $m=0$ and $\delta_{0m} = 0$ for $m \neq 0$. Note that the angular functions ψ_{ml} form a complete orthonormalized system in the space $L_2(\Omega)$, where Ω is a spherical surface having the center at the coordinate origin.

The potentials introduced can be represented by the following expansions in terms of the corresponding solutions to the Laplace equation:

$$\Phi_1^{(1)} = \sum_{m=0}^{\infty}\sum_{l=m}^{\infty} a_{ml}^{(1)} \Psi_{ml}^{(1)}(\vec{r}), \tag{8}$$

$$\Phi_1^{(2)} = \sum_{m=0}^{\infty}\sum_{l=m}^{\infty} a_{ml}^{(2)} \Psi_{ml}^{(1)}(\vec{r}), \tag{9}$$

$$\Phi_2^{(1)} = \sum_{m=0}^{\infty}\sum_{l=m}^{\infty} b_{ml}^{(1)} \Psi_{ml}^{(3)}(\vec{r}). \tag{10}$$

Since the external field is uniform, the expansion of $\Phi_1^{(1)}$ is simplified. When the external field is parallel to the x axis, i.e. $\vec{E}_0 = \vec{i}_x E_0$, the potential is

$$\begin{aligned} \Phi_1^{(1)} &= -xE_0 = -r\sin\theta\cos\varphi E_0 \\ &= -rP_1^1(\cos\theta)\cos\varphi E_0 = a_{11e}^{(1)}\Psi_{11e}^{(1)}(\vec{r}), \end{aligned} \tag{11}$$

or in other words all the coefficients of the expansion of $\Phi_1^{(1)}$ are equal to zero, except for $a_{11e}^{(1)} = -\sqrt{4\pi/3}E_0$.

When the external field is parallel to the y axis, the situation is similar, though the dependence on the azimuthal angle is given by $\sin\varphi$, and Eq. (11) contains the functions $\Psi_{11o}^{(1)}(\vec{r})$ and the coefficient $a_{11o}^{(1)}$.

When the external field is parallel to the z axis, i.e. $\vec{E}_0 = \vec{i}_z E_0$, the potential equals

$$\Phi_1^{(1)} = -zE_0 = -r\cos\theta E_0 = a_{01}^{(1)}\Psi_{01}^{(1)}(\vec{r}), \tag{12}$$

i.e. we have $a_{01}^{(1)} = -\sqrt{4\pi/3}E_0$.

Unknown coefficients of the expansions of $\Phi_1^{(2)}$ and $\Phi_1^{(2)}$ can be found in different ways like in the case of light scattering. Here we apply an analog of the extended boundary condition method, i.e. the corresponding surface integral equations are used. A similar approach has been applied in [18] to solve a two-dimensional (axisymmetric) electrostatic problem. Advantages and limitations of the EBCM method are well known (see, e.g., [19,20]).

The potentials under consideration are solutions to the Laplace Equation (3) and hence satisfy the integral equations found for such solutions (see [21]). After simple transformations (see for more details [18]) we get the following integral equations:

$$(\varepsilon-1)\int_S \left\{ \frac{\partial\Phi_1^{(2)}(\vec{r}')}{\partial n'} G\left(\vec{r}, \vec{r}'\right) \right\} ds' = \begin{cases} \Phi_1^{(1)}(\vec{r}) - \Phi_1^{(2)}(\vec{r}), & \vec{r} \in D, \\ -\Phi_2^{(1)}(\vec{r}), & \vec{r} \in R^3 \backslash \overline{D}, \end{cases} \tag{13}$$

where D is the domain occupied by the particle. The Green function of the scalar Laplace equation for free space is

$$G(\vec{r}, \vec{r}') = 1/4\pi\left|\vec{r} - \vec{r}'\right|, \tag{14}$$

where $\vec{r}$ and $\vec{r}'$ are the radius-vectors to the observation and integration points, respectively. The expansion of the Green function in terms of the spherical functions is well