PERGAMON

Journal of Quantitative Spectroscopy & Radiative Transfer 79–80 (2003) 599–626

Journal of Quantitative Spectroscopy & Radiative Transfer

www.elsevier.com/locate/jqsrt

Light scattering by multilayered nonspherical particles: a set of methods

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Received 1 June 2002; accepted 23 September 2002

Abstract

An original approach to solution of the light scattering problems for axisymmetric particles was developed in our earlier papers. The approach is based on separation of the fields in two specific parts and a proper choice of scalar potentials for each of them. Applications to homogeneous scatterers made first in the framework of the separation of variables method (SVM) and later the extended boundary condition method (EBCM) led to more efficient solutions (at least in the case of the SVM) than the standard ones. The approach was recently applied to formulate new theoretical methods for multilayered axisymmetric particles.

In this paper we further develop and systematically discuss the methods. One of them is a modification of the EBCM and another looking as (and wrongly called) a modification of the SVM is shown to be rather that of the EBCM formulated in spheroidal coordinates. The solutions are now presented in recursive forms. The ranges of applicability of the new methods are considered analytically for the first time in the literature on layered scatterers. The theoretical methods and their program implementations are compared with others available. We note that usage of scalar potentials (a feature of our approach) allowed us consistently to realize the EBCM in spheroidal coordinates. Advantages of this approach in the case of layered spheroidal particles with the confocal layer boundaries are noted.

Earlier we have extended the quasistatic approximation (QSA), being a generalization of the Rayleigh (RA) and Rayleigh-Gans approximations, to layered ellipsoids in the general case of nonconfocal layer boundaries. Here the connection between the QSA and the asymptotic of the scattered field found in the framework of our SVM-like method in the limit of very large aspect ratios of spheroids is discussed. Keeping this fact in mind, the applicability regions of the QSA and RA are comparatively considered for multilayered ellipsoids. We also note that the formulations of the RA and QSA contains a quantity that can be interpreted as the average refractive index of a layered particle and thus gives a new rule of the effective medium theory more appropriate for such scatterers.

Keywords: Light scattering; Inhomogeneous nonspherical particles

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PII: S0022-4073(02)00310-2

1. Introduction

Various natural scatterers are known to have internal structure, and hence the problem of light scattering by inhomogeneous particles is of large interest in different scientific fields—astrophysics, atmosphere and ocean optics, biophysics, etc. In many cases inhomogeneous dust grains can be well represented by multilayered particles. For instance, quasilayers of different composition should form during dust grain evolution in interstellar medium. Particles with many relatively thin layers can be used to model grains with a radially changing refractive index, appearing, for instance, in the case of fractal-like, fluffy aggregates typical of interplanetary media. The model with a large number of very thin layers of several cyclically changing materials opens an efficient way to study effects of composition inhomogeneity expected in cosmic dust grains. We mention only astrophysical applications, but similar examples can be found in other fields as well.

To simulate light scattering by layered particles, when shape effects are of small importance, one usually utilizes the model of multilayered spheres that is based on relatively simple and effective algorithm [1]. This algorithm appears to be applicable practically in the whole range of parameter values after a small improvement. Situation with layered nonspherical particles is much more complex, despite many methods allow one to get solution to the corresponding light scattering problem. In principle, nonspherical scatterers of any structure can be treated by the methods using the representation of the scattering problem in the form of volume integral equation (e.g., the widely used discrete dipole approximation, DDA), the finite difference time domain methods, etc. [2]. The back sides of this universality are strong demands for computer memory and speed which often make computations required by applications impossible.

Layered scatterers could be also treated by the separation of variables method (SVM) and the extended boundary condition method (EBCM) which can better involve the scattering geometry and hence are much faster for some kinds of particle shapes. As a result the methods could allow really extensive calculations, but are not yet well developed—till now detailed consideration was mainly restricted by core-mantle spheroids for the SVM [3–5] and core-mantle axisymmetric particles for the EBCM [6]. Nonspherical particles with three and more layers were studied mainly theoretically, i.e. without computations (see [7,8] for the SVM and [6,9–11] for the EBCM, with an exception being [6] where some illustrative calculations for a three-layered spheroid were done). A universal EBCM-like computer code for layered particles was recently presented in [12], but the paper does not contain results for multilayered particles, estimates of efficiency of the code, and its comparison with others (like the DDA one). It is important here also to distinguish the standard EBCM approach (see, e.g. [13]) from the approach used in [11,12] and other works cited there. In the former expansions of the fields in terms of the spherical wave functions considered in one coordinate system are utilized, in the latter the fields are expanded in terms of finite linear combinations of the spherical wave functions, with combinations being related to different coordinate systems having origins distributed on a closed surface. There is a principal distinction between such single and multipole expansions (different basis) and hence the approaches differ in many important aspects—applicability range, efficiency, etc. In this paper we modify and investigate the standard EBCM approach used in a great number of works (see [2] for a review), and hereafter EBCM means this approach whereas the approach used in [11,12] is called the discrete source method (see [14] for more details).

Besides [11,12] there were many other modifications of the EBCM aimed at overcoming its probably main defect—inability to treat scattering by particles of large eccentricity (see [2] for a review). A perspective way to solve this problem in the case of spheroids could be formulation of the EBCM in spheroidal coordinates (i.e. with expansion of the fields in terms of the spheroidal wave functions), which would better correspond to the scattering geometry than spherical coordinates and functions. For acoustic wave scattering, that was actually done in [15], but for electromagnetic wave scattering, it is impossible in the standard formulation of the EBCM (e.g. [13]) because of nonorthogonality of the spheroidal vector wave functions [16].

The fact that the standard EBCM is not appropriate (expansions of the fields are divergent) for scatterers of large eccentricity is well known, but based mainly on the results of calculations [2,17]. Earlier analytic investigations of the EBCM were summarized in [19] (see also [18,20]). Besides other important results the paper [19] formulates the condition of validity of the Rayleigh hypothesis on convergence of the field expansions everywhere up to the scatterer boundary. Obviously, this condition is the necessary one for applicability of the EBCM in the near zone. A general condition of convergence of the series in the EBCM for the far zone was recently obtained in [21]. This condition is however too abstract to be easily applied to concrete cases. In cite [21] after rather large efforts it was only demonstrated that the condition was satisfied for any ellipsoid. Less abstract analytic investigations of the applicability ranges of EBCM-like methods were made for perfectly conducting and dielectric homogeneous scatterers in [22,23], respectively. These papers give applicability (convergence) conditions for the far zone in the form which allows simple application to Chebyshev particles, spheroids and so on. Note that in contrast to the EBCM another popular approach—the SVM for spheroidal particles was analytically studied in detail long ago [24]. For layered particles, the methods were, however, never analyzed.

Even for such fast methods as the SVM and EBCM, calculations of light scattering by multilayered nonspherical particles are very time consuming. Therefore, various approximate methods (see, e.g. [25] for a review) can be useful in applications. However, one of the most widely used approximations—the Rayleigh approximation (RA) has the same problem as the EBCM—it does not work well for particles whose shape strongly differs from the spherical one. A generalization of the RA—the quasistatic approximation (QSA) apparently avoids this problem for homogeneous spheroidal particles [26]. The QSA was recently extended to multilayered ellipsoids [27], but its applicability range was not discussed, which is rather typical of approximations available for inhomogeneous nonspherical particles.

In this paper we consider a set of exact and approximate methods to calculate the light scattering by multilayered nonspherical (mainly axisymmetric) particles. The corresponding light scattering problem and a general approach used to find exact solutions to the problem are presented in Sections 2 and 3, respectively. Section 4 describes the suggested modification of the EBCM for such particles and gives recursive forms of the solution. Another exact method—a modification of the EBCM in spheroidal coordinates is introduced in Section 5. The next section shows the connection of this method with the QSA and discuss other tightly connected approximations. Section 7 contains analytic estimates of the applicability ranges of the exact and approximate methods and comparison with results of numerical calculations. Conclusions are drawn in the last section.

Let us introduce the notations of the versions of exact methods we mention hereafter and give several general remarks on their relationship. The standard EBCM approach (see, e.g. [13]) is denoted by sEBCM; our modification of the sEBCM [28] by mEBCM and our generalization of the mEBCM for multilayered axisymmetric particles by gmEBCM; the standard SVM approach for spheroids [29] by sSVM; our modification of the sSVM [30] by mSVM and our generalization of the mSVM for multilayered particles by gmSVM. It should be added that the SVM approach with expansions of the fields in terms of the spherical wave functions is equivalent to the sEBCM as was shown in [16]. By analogy, the sSVM, i.e. the standard SVM for spheroids using the spheroidal wave functions for expansions, is equivalent to the sECBM formulated in spheroidal coordinates (sEBCMsc hereafter), i.e. with expansions of the fields in terms of the spheroidal wave functions. Accordingly, the mSVM and mEBCMsc as well as the gmSVM and gmEBCMsc are generally equivalent too (see Section 5 for more details). Note that the SVM approach can be applied not only to spheroids (spheres and infinitely long cylinders) but generally to particles of arbitrary shapes [31]. It should be also noted that in the literature the EBCM was very often called the T-matrix method (TMM). The transition (T) matrix relates the expansion coefficients for the scattered field with those for the incident one and depends only on particle parameters—size, shape, etc. Therefore, the T matrix is a very convenient characteristic in some cases (e.g., when one considers an ensemble of particles) and in several recent papers (e.g. [32–34]) this matrix is derived by methods different from the EBCM. As a result, the usage of the term TMM looks now a bit confusing and in this paper we call the approach EBCM.

2. Formulation of the problem

We consider scattering of a plane wave incident at a n-layered axisymmetric particle. The particle geometry is defined by the layer surface equations

$$r^{(j)}(\theta) = 0, \quad j = 1, 2, \ldots, n, \tag{1}$$

where θ is one of the angles of the spherical coordinate system (r, θ, φ) connected with the particle. The surfaces further called S_j are assumed to have no common points.

The fields in the jth layer confined by the surfaces $r^{(j)}(\theta) = 0$ and $r^{(j+1)}(\theta) = 0$ are denoted by $\vec{E}^{(j+1)}, \vec{H}^{(j+1)}$. Thus, $j = 1$ corresponds to the outermost layer (a mantle of the particle) and $j = n$ to the innermost layer (a core). As in the case of a homogeneous particle ($n = 1$), $\vec{E}^{(0)}, \vec{H}^{(0)}$ and $\vec{E}^{(1)}, \vec{H}^{(1)}$ are the incident and scattered fields, respectively.

An arbitrary polarized plane electromagnetic wave, incident at the angle α to the symmetry axis of the particle, can be represented by a superposition of the waves of two kinds:

(a) TE mode

$$\begin{aligned} \vec{E}^{(0)}(\vec{r}) &= -\vec{i_y} \exp[\mathrm{i}k_1(x \sin\alpha + z \cos\alpha)], \\ \vec{H}^{(0)}(\vec{r}) &= \sqrt{\frac{\varepsilon_1}{\mu_1}} (\vec{i_x} \cos\alpha - \vec{i_z} \sin\alpha) \exp[\mathrm{i}k_1(x \sin\alpha + z \cos\alpha)], \end{aligned} \tag{2}$$

(b) TM mode

$$\begin{aligned} \vec{E}^{(0)}(\vec{r}) &= (\vec{i_x} \cos\alpha - \vec{i_z} \sin\alpha) \exp[\mathrm{i}k_1(x \sin\alpha + z \cos\alpha)], \\ \vec{H}^{(0)}(\vec{r}) &= \sqrt{\frac{\varepsilon_1}{\mu_1}} \vec{i_y} \exp[\mathrm{i}k_1(x \sin\alpha + z \cos\alpha)], \end{aligned} \tag{3}$$

where $(\vec{i_x}, \vec{i_y}, \vec{i_z})$ are the unit vectors of the Cartesian coordinate system, whose z-axis coincides with the symmetry axis of the particle, $\vec{r} = (x, y, z)$, ε_1 and μ_1 are the dielectric permittivity and magnetic permeability outside the particle, k_1 is the wavenumber.

The problem is to solve Maxwell's equations for each layer ($j = 1, 2, \ldots, n$)

$$\vec{E^{(j)}}(\vec{r}) = -\frac{1}{\mathrm{i}\varepsilon_j k_0}\vec{\nabla} \times \vec{H^{(j)}}(\vec{r}), \quad \vec{H^{(j)}}(\vec{r}) = \frac{1}{\mathrm{i}\mu_j k_0}\vec{\nabla} \times \vec{E^{(j)}}(\vec{r}) \tag{4}$$

with the boundary conditions at each layer surface

$$\left.\begin{aligned} \vec{E}^{(j)}(\vec{r}) \times \vec{n_j} &= \vec{E}^{(j+1)}(\vec{r}) \times \vec{n_j} \\ \vec{H}^{(j)}(\vec{r}) \times \vec{n_j} &= \vec{H}^{(j+1)}(\vec{r}) \times \vec{n_j} \end{aligned}\right\}_{\vec{r} \in S_j} \tag{5}$$

and the radiation condition at infinity ($r \to \infty$)

$$\lim r \left(\frac{\partial \vec{E^{(1)}}(\vec{r})}{\partial r} - \mathrm{i}k_1 \vec{E^{(1)}}(\vec{r}) \right) = 0, \quad \lim r \left(\frac{\partial \vec{H^{(1)}}(\vec{r})}{\partial r} - \mathrm{i}k_1 \vec{H^{(1)}}(\vec{r}) \right) = 0. \tag{6}$$

Here ε_j and μ_j are the dielectric permittivity and magnetic permeability, respectively, $k_0 = \omega/c$ is the wavenumber in vacuum, ω the radiation frequency, c the velocity of light in vacuum, $\vec{n_j}$ the outward normal to the jth layer surface S_j, $\vec{r}$ the radius-vector, $r = |\vec{r}|$. We assume that the time dependence of the electromagnetic fields is given by the factor $\exp(-\mathrm{i}\omega t)$.

3. Description of the approach

To find solution to the described problem, we apply the approach earlier suggested for homogeneous axisymmetric scatterers [24]. The main features of the approach are as follows:

1. All the fields are divided in two parts—an *axisymmetric* one that does not depend on the azimuthal angle φ and an *nonaxisymmetric* one whose averaging over φ gives zero

$$\vec{E}^{(j)}(\vec{r}) = \vec{E}^{(j)}_{\mathrm{A}}(\vec{r}) + \vec{E}^{(j)}_{\mathrm{N}}(\vec{r}), \quad \vec{H}^{(j)}(\vec{r}) = \vec{H}^{(j)}_{\mathrm{A}}(\vec{r}) + \vec{H}^{(j)}_{\mathrm{N}}(\vec{r}), \tag{7}$$

where $j = 0, 1, \ldots, n+1$. The possibility of such a representation of the fields was considered in [35]. The light scattering problems for the parts can be solved independently. Such a separation is possible because of commutation of the operator corresponding to the diffraction problem and the operator $L_z = \partial/\partial\varphi$ (see [35] for more details). Thus, the problem under consideration can be uncoupled relative to the azimuthal angle φ, i.e. each component of the Fourier expansion can be found separately.

2. Proper scalar potentials are chosen for each of the field parts. For the axisymmetric parts, we apply the potentials analogous to the Abraham potentials for spheroids which are known to simplify solutions for such particles [36]. For the nonaxisymmetric parts, we utilize combinations of the Debye potentials used in solutions for spheres and z-components of the Hertz vectors used for infinitely long cylinders.

The approach was found highly efficient for solution of the light scattering problem for spheroids by the separation of variables method [30]. Note that only the nonaxisymmetric parts and their potentials were used in the modification of the approach in [8]. Such a variant has more simple formulation, but computationally may be less favorite.

4. Modification of the EBCM

The described approach was applied to find solution to the light scattering problem for homogeneous particles in the framework of the EBCM in [28,37,38]. We have also generalized that solution (mEBCM) for the case of multilayered axisymmetric scatterers [10]. Here we briefly describe the main steps of the generalized solution to be able to reveal and discuss differences of the suggested modification of the EBCM and other methods. For the sake of simplicity, solutions for the axisymmetric and nonaxisymmetric parts are considered separately, though they are similar in many details.

4.1. Axisymmetric parts of the fields

To construct the scalar potentials to these parts inside each layer we use the azimuthal components of the fields

$$p^{(j)}(\vec{r}) = E^{(j)}_{A,\varphi}(\vec{r})\cos\varphi, \quad q^{(j)}(\vec{r}) = H^{(j)}_{A,\varphi}(\vec{r})\cos\varphi, \tag{8}$$

where $j = 0, 1, \ldots, n+1$ and the potentials p, q satisfy the scalar Helmholtz equation

$$\Delta q^{(j)}(\vec{r}) + k_j^2 q^{(j)}(\vec{r}) = 0 \tag{9}$$

with $k_j = \sqrt{\varepsilon_j \mu_j} k_0$. Other components of the fields can be expressed via the potentials using Maxwell's equations:

$$E^{(j)}_{A}(\vec{r}) = \left(\frac{-1}{\mathrm{i}\varepsilon_j k_0 r \sin\theta\cos\varphi} \frac{\partial(\sin\theta\, q^{(j)})}{\partial\theta}, \frac{1}{\mathrm{i}\varepsilon_j k_0 r\cos\varphi} \frac{\partial(r q^{(j)})}{\partial r}, \frac{p^{(j)}}{\cos\varphi} \right),$$

$$H^{(j)}_{A}(\vec{r}) = \left(\frac{1}{\mathrm{i}\mu_j k_0 r \sin\theta\cos\varphi} \frac{\partial(\sin\theta\, p^{(j)})}{\partial\theta}, \frac{-1}{\mathrm{i}\mu_j k_0 r\cos\varphi} \frac{\partial(r p^{(j)})}{\partial r}, \frac{q^{(j)}}{\cos\varphi} \right). \tag{10}$$

Easy to see that the potentials p and q are connected with the TE and TM modes, respectively. The equations for p are generally similar to those for q, and below we mention the TE mode and the potentials p only if an essential difference appears.

For each layer, we represent the scalar potentials as sums

$$q^{(j)}(\vec{r}) = q_1^{(j)}(\vec{r}) + q_2^{(j)}(\vec{r}), \tag{11}$$

where $q_1^{(j)}$ has no peculiarity at the origin of the coordinate system, $q_2^{(j)}$ satisfies the radiation condition at infinity. Note that $q_1^{(n+1)} = q^{(n+1)}$, $q_2^{(n+1)} = 0$ and Eq. (11) can be considered for $j = 1, 2, \ldots, n+1$, if one uses the following notations: $q_1^{(1)} = q^{(0)}$, $q_2^{(1)} = q^{(1)}$.

The introduced quantities allow one to write the surface integral equation equivalent to the scalar wave equation (see, e.g. [39]) in a more convenient way:

$$\int_{S_j} \left\{ q^{(j)}(\vec{r}') \frac{\partial G(k_j,\vec{r},\vec{r}')}{\partial n} - \frac{\partial q^{(j)}(\vec{r}')}{\partial n} G(k_j,\vec{r},\vec{r}') \right\} \mathrm{d}S' = \begin{cases} -q_1^{(j)}(\vec{r}), & \vec{r} \in D_j, \\ q_2^{(j)}(\vec{r}), & \vec{r} \in R^3 \setminus \bar{D}_j, \end{cases} \tag{12}$$

where $G(k,\vec{r},\vec{r}')$ is the free-space Green function, D_j the domain confined by the surface S_j ($j = 1,2,\dots,n$). Then the potential for a layer can be expressed via the potential for the previous one. As a result we shall get the solution in the form, where quantities for each layer are totally separated.

The boundary conditions (5) for the potentials can be rewritten as follows:

$$\left.\begin{aligned} & p^{(j)} = p^{(j+1)}, \\ & \frac{\partial p^{(j)}}{\partial n_j} = \frac{\mu_j}{\mu_{j+1}} \frac{\partial p^{(j+1)}}{\partial n_j} + \left(\frac{\mu_j}{\mu_{j+1}} - 1 \right) \frac{1}{\sqrt{r^2 + r_{\theta'}^2}} \left(1 - \frac{r'_\theta}{r} \operatorname{ctg}\theta \right) p^{(j+1)}, \\ & q^{(j)} = q^{(j+1)}, \\ & \frac{\partial q^{(j)}}{\partial n_j} = \frac{\varepsilon_j}{\varepsilon_{j+1}} \frac{\partial q^{(j+1)}}{\partial n_j} + \left(\frac{\varepsilon_j}{\varepsilon_{j+1}} - 1 \right) \frac{1}{\sqrt{r^2 + r_{\theta'}^2}} \left(1 - \frac{r'_\theta}{r} \operatorname{ctg}\theta \right) q^{(j+1)}, \end{aligned}\right\}_{\vec{r} \in S_j}, \tag{13}$$

where r'_θ is the derivative of $r_j(\theta)$ with respect to the spherical angle θ, and $j = 1,2,\dots,n$.

After the substitution of the conditions (13) in Eq. (12) one gets

$$\begin{aligned} \int_{S_j} \Bigg\{ & q^{(j+1)}(\vec{r}') \frac{\partial G(k_j,\vec{r},\vec{r}')}{\partial n} - \left[\frac{\varepsilon_j}{\varepsilon_{j+1}} \frac{\partial q^{(j+1)}(\vec{r}')}{\partial n} + \left(\frac{\varepsilon_j}{\varepsilon_{j+1}} - 1 \right) \frac{1}{\sqrt{(r')^2 + [(r')'_{\theta'}]^2}} \right. \\ & \left. \times \left(1 - \frac{(r')'_{\theta'}}{r'} \operatorname{ctg}\theta' \right) q^{(j+1)}(\vec{r}') \right] G(k_j,\vec{r},\vec{r}') \Bigg\} \mathrm{d}S' = \begin{cases} -q_1^{(j)}(\vec{r}), & \vec{r} \in D_j, \\ q_2^{(j)}(\vec{r}), & \vec{r} \in R^3 \setminus \bar{D}_j. \end{cases} \end{aligned} \tag{14}$$

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

$$\begin{matrix} p_1^{(j)}(\vec{r}) \\ q_1^{(j)}(\vec{r}) \end{matrix} = \sum_{l=1}^{\infty} \begin{matrix} a_{1,l}^{(j)} \\ b_{1,l}^{(j)} \end{matrix} j_l(k_j r)\, P_l^1(\cos\theta) \cos\varphi, \tag{15}$$

where $j_l(k_j r)$ are the spherical Bessel functions, $P_l^1(\cos\theta)$ the associated Legendre functions, $j = 1,2,\dots,n+1$. The potentials $p_2^{(j)}, q_2^{(j)}$ are expanded in the same way, but $j_l(k_j r)$ are replaced by the Hankel functions of the first kind $h_l^{(1)}(k_j r)$. The spherical harmonic expansion of the free-space Green function is well known (see, e.g. [40]).

All the expansions are substituted into the surface integral equations (14). Due to orthogonality of the spherical wave functions, one gets two infinite systems of algebraic equations relative to the expansion coefficients of the scattered and internal field potentials. Solution of the systems gives the coefficients for the scattered field, $\vec{a}^{(1)} = \{a_{2,l}^{(1)}\}_{l=1}^{\infty}$, in the form typical of the EBCM

$$\vec{a}^{(1)} = A_2 A_1^{-1} \vec{a}^{(0)}, \tag{16}$$

where $\vec{a}^{(0)} = \{a_{1,l}^{(0)}\}_{l=1}^{\infty}$ are known coefficients for the incident field (a plane wave). The matrices A_1 and A_2 are determined as follows:

$$\begin{pmatrix} A_1 \\ A_2 \end{pmatrix} = \begin{pmatrix} -A_{hj}^{(1)} & -A_{hh}^{(1)} \\ A_{jj}^{(1)} & A_{jh}^{(1)} \end{pmatrix} \cdots \begin{pmatrix} -A_{hj}^{(n-1)} & -A_{hh}^{(n-1)} \\ A_{jj}^{(n-1)} & A_{jh}^{(n-1)} \end{pmatrix} \begin{pmatrix} -A_{hj}^{(n)} \\ A_{jj}^{(n)} \end{pmatrix}. \tag{17}$$

Here $A^{(j)}$ are the matrices whose elements are surface integrals of products of the spherical wave functions and their derivatives calculated for the jth layer, for instance

$$\begin{aligned}(A_{hj}^{(j)})_{ln} = \frac{\mathrm{i}(2l+1)}{2l(l+1)} \int_0^{\pi} \Bigg\{ & k_j^2 r_j^2 \left[h_l^{(1)'}(k_j r_j) j_n(k_{j+1} r_j) - \frac{\varepsilon_j}{\varepsilon_{j+1}} \frac{k_{j+1}}{k_j} h_l^{(1)}(k_j r_j) j_n'(k_{j+1} r_j) \right] \\ & \times P_l^1(\cos\theta) P_n^1(\cos\theta) \sin\theta + k_j (r_j)_\theta' \sin^2\theta \Bigg[P_l^{1'}(\cos\theta) P_n^1(\cos\theta) \\ & - \frac{\varepsilon_j}{\varepsilon_{j+1}} P_l^1(\cos\theta) P_n^{1'}(\cos\theta) \Bigg] h_l^{(1)}(k_j r_j) j_n(k_{j+1} r_j) - \left(\frac{\varepsilon_j}{\varepsilon_{j+1}} - 1 \right) \\ & \times (k_j r_j \sin\theta - k_j (r_j)_\theta' \cos\theta) h_l^{(1)}(k_j r_j) j_n(k_{j+1} r_j) P_l^1(\cos\theta) P_n^1(\cos\theta) \Bigg\} \, \mathrm{d}\theta. \end{aligned} \tag{18}$$

The subscripts j, h of $A^{(j)}$ matrices show what radial functions are used in the corresponding places in the integrals (18)—the spherical Bessel (j) or Hankel (h) one.

4.2. Nonaxisymmetric parts of the fields

The scalar potentials selected for these parts are superpositions of the vertical components of the Hertz vector $U^{(j)}$ and the Debye potentials $V^{(j)}$ ($j = 0, 1, \ldots, n$). For instance, for TM mode we have

$$\vec{E}_{\mathrm{N}}^{(j)} = -\frac{1}{\mathrm{i}\varepsilon_j k_0} \vec{\nabla} \times \vec{\nabla} \times (U^{(j)} \vec{i}_z + V^{(j)} \vec{r}), \tag{19}$$

$$\vec{H}_{\mathrm{N}}^{(j)} = \vec{\nabla} \times (U^{(j)} \vec{i}_z + V^{(j)} \vec{r}).$$

In the same way as in Section 4.1 we represent the scalar potentials for each layer as sums

$$U^{(j)}(\vec{r}) = U_1^{(j)}(\vec{r}) + U_2^{(j)}(\vec{r}), \quad V^{(j)}(\vec{r}) = V_1^{(j)}(\vec{r}) + V_2^{(j)}(\vec{r}). \tag{20}$$

The boundary conditions for the TM mode can be written as follows:

$$\left.\begin{aligned}
U^{(j)} &= U^{(j+1)},\\
V^{(j)} &= V^{(j+1)},\\
\frac{\partial U^{(j)}}{\partial n} &= \frac{\partial U^{(j+1)}}{\partial n} + \left(\frac{\varepsilon_j}{\varepsilon_{j+1}} - 1\right)\frac{r'_\theta}{r\sin\theta\sqrt{r^2+r^2_{\theta'}}}\left[r\cos\theta\frac{\partial U^{(j+1)}}{\partial r}\right.\\
&\qquad \left. -\sin\theta\frac{\partial U^{(j+1)}}{\partial\theta} + r^2\frac{\partial V^{(j+1)}}{\partial r} + rV^{(j+1)}\right],\\
\frac{\partial V^{(j)}}{\partial n} &= \frac{\partial V^{(j+1)}}{\partial n} + \left(\frac{\varepsilon_j}{\varepsilon_{j+1}} - 1\right)\frac{\left(r'_\theta\cos\theta - r\sin\theta\right)}{r^2\sin\theta\sqrt{r^2+r^2_{\theta'}}}\left[r\cos\theta\frac{\partial U^{(j+1)}}{\partial r}\right.\\
&\qquad \left. -\sin\theta\frac{\partial U^{(j+1)}}{\partial\theta} + r^2\frac{\partial V^{(j+1)}}{\partial r} + rV^{(j+1)}\right],
\end{aligned}\right\}_{\vec r\in S_j} . \tag{21}$$

Substitution of the corresponding boundary conditions in the surface integral equations (12) leads to the integral equations well resembling those for the axisymmetric parts (see Eq. (14)).

The potentials are expanded in terms of the spherical wave functions

$$\begin{matrix} U_1^{(j)}(\vec r) \\ V_1^{(j)}(\vec r) \end{matrix} = \sum_{m=1}^{\infty}\sum_{l=m}^{\infty} \begin{matrix} a_{1,ml}^{(j)} \\ b_{1,ml}^{(j)} \end{matrix} \; j_l(k_j r)\, P_l^m(\cos\theta)\cos m\varphi. \tag{22}$$

The expressions for the potentials with the subscript 2 are the same after the replacement of $j_l(k_j r)$ with $h_l^{(1)}(k_j r)$.

Substitution of the expansions into the surface integral equations gives for each m two infinite systems of algebraic equations relative to the coefficients of the potential expansions. Solution of the systems provides the coefficients for the scattered field $\vec a_m^{(1)} = \{a_{2,ml}^{(1)}\}_{l=1}^{\infty}$, $\vec b_m^{(1)} = \{b_{2,ml}^{(1)}\}_{l=1}^{\infty}$ $(m \geqslant 1)$ in the form (16)–(17) with the only difference—the matrices $A^{(j)}$ are now twice as large and have the block structure

$$A_{hj}^{(j)} = \begin{pmatrix} \alpha_{hj,1}^{(j)} & \beta_{hj,1}^{(j)} \\ \alpha_{hj,2}^{(j)} & \beta_{hj,2}^{(j)}, \end{pmatrix}, \tag{23}$$

where $\alpha_{hj,i}^{(j)}$, $\beta_{hj,i}^{(j)}$ are the matrices whose elements are surface integrals of products of the spherical wave functions and their derivatives calculated for the jth layer (see [10] for more details).

The systems arising for axisymmetric and nonaxisymmetric parts were investigated analytically and numerically in the case of homogeneous particles [23]. It was found that they had similar properties and affected the range of applicability of the method nearly in the same way.

4.3. Recursive forms of the solution

It is important to note that the most essential part of the solution— Eq. (17) can be rewritten in the recursive form

$$\begin{pmatrix} A_1^{(n+1)} \\ A_2^{(n+1)} \end{pmatrix} = \begin{pmatrix} -A_{hj}^{(1)} - A_{hh}^{(1)} \\ A_{jj}^{(1)} \; A_{jh}^{(1)} \end{pmatrix} \begin{pmatrix} A_1^{(n)} \\ A_2^{(n)}, \end{pmatrix}, \tag{24}$$

where the right-hand side vector contains the values of A_1, A_2 for a given n-layered particle, the matrix corresponds to a new outer layer, and the left-hand side vector gives the values of A_1, A_2 for the $(n+1)$-layered particle formed in such a way.

Eq. (24) can be rewritten in another way

$$T_{n+1} = (A_{jj}^{(n+1)} + A_{jh}^{(1)} T_n)(A_{hj}^{(n+1)} + A_{hh}^{(1)} T_n)^{-1}, \tag{25}$$

where $T_n = A_2^{(n)}(A_1^{(n)})^{-1}$. Eq. (25) is equivalent to that obtained earlier for multilayered axisymmetric particles in [6]. Although Eq. (24) looks less exiting, it should be preferable to Eq. (25) as the former needs only one matrix inversion (after multiplication of A-matrices in $T_{n+1} = A_2^{(n+1)}(A_1^{(n+1)})^{-1}$) in contrast with the latter that requires inversions for each layer (to find each T_n starting with $n = 1$) and one more at the last step.

5. Modification of the EBCM in spheroidal coordinates and the SVM

The approach described in Sections 3 and 4 has been used in [7] to find the theoretical solution of the light scattering problem defined in Section 2 in the framework of the EBCM formulated in spheroidal coordinates (i.e. with the potentials expanded in terms of the spheroidal wave functions, etc.). Note that such a version of the EBCM for spheroids only weakly differs from the SVM (see also [16]) as the separation of variables in the boundary conditions for spheroids is impossible and the light scattering problem in the SVM is reduced to solution of infinite algebraic systems similar to those arising in the EBCM with spheroidal coordinates (a difference may appear in the boundary conditions as it will be seen below). Therefore, this variant of the EBCM can also be considered as a SVM-like method. For homogeneous and core-mantle spheroidal particles, our approach has been applied to the SVM in [24,30,5], respectively (mSVM solutions). It should be added that as far as we know first the problem of electromagnetic scattering was consistently solved within the EBCM formulated in spheroidal coordinates in [7] (mEBCMsc solution).

To use in the full manner the advantages of expansions in terms of the spheroidal wave function, we assume that all layer boundaries are confocal, i.e. for all j, $r^{(j)}(\theta)$ are coordinate surfaces of the same spheroidal coordinate system (ξ, η, φ). It means that the major a_j and minor b_j semiaxes of the spheroidal surfaces confining the layers satisfy the condition

$$a_1^2 - b_1^2 = a_2^2 - b_2^2 = \cdots = a_n^2 - b_n^2 = \left(\frac{d}{2}\right)^2, \tag{26}$$

where d is the focal distance of the spheroids.

As in Sections 3 and 4 we divide the fields in the two parts and introduce the scalar potentials p, q, U, V. The scalar Helmholtz equation (9) and the equivalent surface integral equation (12) are written in the spheroidal coordinates as well as the boundary conditions (see also Eq. (39) below). The spheroidal wave functions are used in expansions of the potentials and the free-space Green function. For instance, for prolate spheroidal boundaries of layers we have (cf. Eq. (15))

$$\begin{matrix} p_1^{(j)}(\vec{r}) \\ q_1^{(j)}(\vec{r}) \end{matrix} = \sum_{l=1}^{\infty} \begin{matrix} a_{1,l}^{(j)} \\ b_{1,l}^{(j)} \end{matrix} R_{1l}^{(1)}(c_j, \xi) S_{1l}(c_j, \eta) \cos\varphi, \tag{27}$$

$$\begin{matrix} p_2^{(j)}(\vec{r}) \\ q_2^{(j)}(\vec{r}) \end{matrix} = \sum_{l=1}^{\infty} \begin{matrix} a_{2,l}^{(j)} \\ b_{2,l}^{(j)} \end{matrix} R_{1l}^{(3)}(c_j, \xi)\ S_{1l}(c_j, \eta) \cos\varphi, \tag{28}$$

where $R_{1l}^{(1),(3)}(c_j, \xi)$ are the prolate radial spheroidal functions of the first or third kinds, $S_{1l}(c_j, \eta)$ the prolate angular spheroidal functions with the normalization factor $N_{1l}(c_j)$ [41], and $c_j = k(d_j/2)$.

After substitution of the expansions in the equation analogous to Eq. (14), due to orthogonality of the spheroidal functions one gets an infinite system of linear algebraic equations like Eq. (16). The integrals in the matrix elements in the analogs of the A_1, A_2 matrices will not contain the radial spheroidal functions, since

$$\frac{\partial}{\partial n}\, \mathrm{d}S = \frac{d}{2}(\xi^2 - 1)\frac{\partial}{\partial \xi}\, \mathrm{d}\eta\, \mathrm{d}\varphi \tag{29}$$

and for example, for the axisymmetric parts, one has (cf. Eqs. (16)–(18))

$$\vec{a}_r^{(1)} = A_2 A_1^{-1}\, \vec{a}_r^{(0)}, \tag{30}$$

where the vectors $\vec{a}_r^{(j)} = \left\{ a_{r1,l}^{(j)} + a_{r2,l}^{(j)} \right\}_{l=1}^{\infty}$ and

$$a_{r1,l}^{(j)} = a_{1,l}^{(j)} R_{1l}^{(1)}(c_j, \xi_j) N_{1l}(c_j), \quad a_{r2,l}^{(j)} = a_{2,l}^{(j)} R_{1l}^{(3)}(c_j, \xi_j) N_{1l}(c_j). \tag{31}$$

The matrix elements in the analog of Eq. (17) are

$$A_{hj}^{(j)} = W_j \left\{ R_j^{(3)}\ S_{j,j+1} - \frac{\mu_j}{\mu_{j+1}} S_{j,j+1}\, \tilde{R}_{j+1}^{(1)} - \left(\frac{\mu_j}{\mu_{j+1}} - 1 \right) \frac{\xi_j}{\xi_j^2 - f} S_{j,j+1} \right\} P_j^{(1)}, \tag{32}$$

$$A_{hh}^{(j)} = W_j \left\{ R_j^{(3)}\ S_{j,j+1} - \frac{\mu_j}{\mu_{j+1}} S_{j,j+1}\ \tilde{R}_{j+1}^{(3)} - \left(\frac{\mu_j}{\mu_{j+1}} - 1 \right) \frac{\xi_j}{\xi_j^2 - f} S_{j,j+1} \right\} P_j^{(3)}, \tag{33}$$

$$A_{jj}^{(j)} = W_j \left\{ R_j^{(1)}\ S_{j,j+1} - \frac{\mu_j}{\mu_{j+1}} S_{j,j+1}\ \tilde{R}_{j+1}^{(1)} - \left(\frac{\mu_j}{\mu_{j+1}} - 1 \right) \frac{\xi_j}{\xi_j^2 - f} S_{j,j+1} \right\} P_j^{(1)}, \tag{34}$$

$$A_{jh}^{(j)} = W_j \left\{ R_j^{(1)}\ S_{j,j+1} - \frac{\mu_j}{\mu_{j+1}} S_{j,j+1}\ \tilde{R}_{j+1}^{(3)} - \left(\frac{\mu_j}{\mu_{j+1}} - 1 \right) \frac{\xi_j}{\xi_j^2 - f}\ S_{j,j+1} \right\}\ P_j^{(3)}, \tag{35}$$

where $f=-1$ for oblate spheroids and 1 for prolate ones, and the subscripts j,h could be replaced by 1,3 to show better the kind of the radial functions used. The diagonal matrices used are

$$
\begin{aligned}
P_j^{(i)} &= \left\{ R_{1l}^{(i)}(c_{j+1},\xi_j)/R_{1l}^{(i)}(c_{j+1},\xi_{j+1})\delta_{nl} \right\}_{n,l=1}^{\infty},\\
R_j^{(i)} &= \left\{ R_{1l}^{(i)\prime}(c_j,\xi_j)/R_{1l}^{(i)}(c_j,\xi_j)\delta_{nl} \right\}_{n,l=1}^{\infty},\\
\tilde{R}_{j+1}^{(i)} &= \left\{ R_{1l}^{(i)\prime}(c_{j+1},\xi_j)/R_{1l}^{(i)}(c_{j+1},\xi_j)\delta_{nl} \right\}_{n,l=1}^{\infty},\\
W_j &= -(R_j^{(3)}-R_j^{(1)})^{-1} = \left\{ ic_j(\xi_j^2-f)\; R_{1l}^{(1)}(c_j,\xi_j)\, R_{1l}^{(3)}(c_j,\xi_j)\,\delta_{nl} \right\}_{n,l=1}^{\infty},
\end{aligned}
\tag{36}
$$

where δ_{nl} is the Kronecker symbol. The elements of the matrix $S_{i,j}=\{s_{nl}(c_i,c_j)\}_{n,l=1}^{\infty}$ are integrals of products of the angular spheroidal functions and can be written as series including the coefficients of their expansions in terms of the Legendre polynomials d_k^{mn} (see [30] for more details)

$$
\begin{aligned}
s_{nl}(c_i,c_j) &= \int_{-1}^{1} \bar{S}_{1n}(c_i,\eta)\bar{S}_{1l}(c_j,\eta)\,\mathrm{d}\eta\\
&= N_{1n}^{-1}(c_i)N_{1l}^{-1}(c_j)\sum_{k=0,1}^{\infty}\frac{2(k+1)(k+2)}{2k+3}\,d_k^{1n}(c_i)\,d_k^{1l}(c_j),
\end{aligned}
\tag{37}
$$

where $\bar{S}_{1n}(c,\eta)$ are normalized angular spheroidal functions. As a result numerical calculations of the matrix elements with high accuracy is not a problem.

For nonaxisymmetric parts, we get equations similar to those described above. Solution for both parts can be formulated in the recursive forms (24), (25) as well.

It should be noted that our modification of the SVM (mSVM) for homogeneous [30] and core-mantle [5] spheroids differs from the above-described modification of the EBCM in spheroidal coordinates generalized for layered particles (gmEBCMsc) mainly by another formulation of the boundary conditions. For the axisymmetric parts, this difference is small, and the algebraic systems are the same if one excludes the Wronskian for the radial spheroidal functions. However, for the nonaxisymmetric parts, the difference (introduced by us to get a more convenient form of solution) is essential. For instance, for the TM mode, we have:

for the mSVM (see [5])

$$
\left.
\begin{aligned}
U^{(j)} &= U^{(j+1)},\\
V^{(j)} &= V^{(j+1)},\\
\frac{\partial}{\partial\xi}\left(\xi U^{(j)} + f\,\frac{d}{2}\,\eta V^{(j)}\right) &= \frac{\partial}{\partial\xi}\left(\xi U^{(j+1)} + f\,\frac{d}{2}\,\eta V^{(j+1)}\right),\\
\frac{1}{\varepsilon_j}\,\frac{\partial}{\partial\xi}\left(\eta U^{(j)} + \frac{d}{2}\,\xi V^{(j)}\right) &= \frac{1}{\varepsilon_{j+1}}\left[\frac{\partial}{\partial\xi}\left(\eta U^{(j+1)} + \frac{d}{2}\,\xi V^{(j+1)}\right)\right.\\
&\quad \left. + \left(1-\frac{c_{j+1}^2}{c_j^2}\right)\frac{1-\eta^2}{\xi^2-f}\,\frac{\partial}{\partial\eta}\left(\xi U^{(j+1)} + f\,\frac{d}{2}\,\eta V^{(j+1)}\right)\right],
\end{aligned}
\right\}_{\xi=\xi_j}
\tag{38}
$$

and for the gmEBCMsc

$$\left.\begin{aligned} U^{(j)} &= U^{(j+1)}, \\ V^{(j)} &= V^{(j+1)}, \\ \frac{\partial}{\partial\xi}U^{(j)} &= \frac{\varepsilon_j}{\varepsilon_{j+1}}\frac{\partial}{\partial\xi}U^{(j+1)} - \left(\frac{\varepsilon_j}{\varepsilon_{j+1}} - 1\right)\left[\frac{\xi^2}{\xi^2 - f\eta^2}\frac{\partial}{\partial\xi}U^{(j+1)} + \frac{f\xi\eta}{\xi^2 - f\eta^2}\frac{\partial}{\partial\xi}\frac{d}{2}V^{(j+1)}\right] \\ &\quad + \left(1 - \frac{\varepsilon_j}{\varepsilon_{j+1}}\right)\frac{f\eta}{\xi^2 - f\eta^2}\left[\frac{1-\eta^2}{\xi^2 - f}\frac{\partial}{\partial\eta}\left(\xi U^{(j+1)} + f\eta\frac{d}{2}V^{(j+1)}\right) + \frac{d}{2}V^{(j+1)}\right], \\ \frac{d}{2}\frac{\partial}{\partial\xi}V^{(j)} &= \frac{d}{2}\frac{\partial}{\partial\xi}V^{(j+1)} + \left(\frac{\varepsilon_j}{\varepsilon_{j+1}} - 1\right)\left[\frac{\xi\eta}{\xi^2 - f\eta^2}\frac{\partial}{\partial\xi}U^{(j+1)} + \frac{\xi^2}{\xi^2 - f\eta^2}\frac{\partial}{\partial\xi}\frac{d}{2}V^{(j+1)}\right] \\ &\quad - \left(1 - \frac{\varepsilon_{j+1}}{\varepsilon_j}\right)\frac{\xi}{\xi^2 - f\eta^2}\left[\frac{1-\eta^2}{\xi^2 - f}\frac{\partial}{\partial\eta}\left(\xi U^{(j+1)} + f\eta\frac{d}{2}V^{(j+1)}\right) + \frac{d}{2}V^{(j+1)}\right]. \end{aligned}\right\}_{\xi=\xi_j} \quad (39)$$

In the mSVM the first two equations in Eq. (38) were used to exclude two series of unknown coefficients in the last two equations. As a result for homogeneous particles one gets more simple algebraic systems (see [30]). However, for multilayered particles the order of truncated systems grows then proportionally to the number of layers (see [5]), because the potentials cannot be presented in the form (11) and the integral identities analogous to Eq. (12) cannot be used.

In the gmEBCMsc the boundary conditions are formulated in such a way that the potentials and their normal derivatives for a layer could be expressed via those for the previous layer (see Eq. (39) which is generally equivalent to Eq. (38)). Then the integral identities (12) allow one partly to resolve the appearing infinite algebraic systems (using Eq. (11)) and to present the final system in the form (16)–(17). Note that in contrast with a recent paper developing a version of the mSVM for layered spheroids [8], we present the solution in the form of systems of *linear* algebraic equations.

6. Quasistatic and other approximations

For very elongated and flattened homogeneous spheroids (the aspect ratio $a/b \to \infty$ and the parameter $c_1 = \mathrm{O}(1)$), the infinite systems arising in the mSVM (and mEBCMsc) were resolved analytically in [30]. It was possible as in this limit the matrices $R_j^{(1)}$, $R_j^{(3)}$ and others (see Section 5) essentially simplified. For example, taking into account the asymptotic behavior of the radial spheroidal functions one gets for prolate spheroids with $b/a \ll 1$

$$R_j^{(1)} = \left(\frac{a}{b}\right)^2\left[1 + \mathrm{O}\left(\frac{b}{a}\right)^2\right]I, \quad R_j^{(3)} = -\left(\frac{a}{b}\right)^2\left[1 + \mathrm{O}\left(\frac{b}{a}\right)^2\right]I, \quad (40)$$

where I is the unit matrix.

In the far zone ($r \to \infty$) the following asymptotics of the scattered field in the case of the small parameter b/a were obtained for a prolate spheroid:

$$\vec{E}^{(1)}_{\mathrm{TE}}(\varphi,\theta) = \frac{\exp \mathrm{i}k_1 r}{k_1 r}\left(\frac{b}{a}\right)^2 \frac{\varepsilon-1}{\varepsilon+1}(T_1 \cos\varphi\, \vec{i}_\varphi + T_2 \sin\varphi\, \vec{i}_\theta),$$

$$\vec{E}^{(1)}_{\mathrm{TM}}(\varphi,\theta) = \frac{\exp \mathrm{i}k_1 r}{k_1 r}\left(\frac{b}{a}\right)^2 \left[\frac{\varepsilon-1}{\varepsilon+1}T_3 \sin\varphi\, \vec{i}_\varphi + \left(\frac{\varepsilon-1}{2}T_4 + \frac{\varepsilon-1}{\varepsilon+1}T_5\cos\varphi\right)\vec{i}_\theta\right] \tag{41}$$

and for an oblate one

$$\vec{E}^{(1)}_{\mathrm{TE}}(\varphi,\theta) = \frac{\exp \mathrm{i}k_1 r}{k_1 r}\left(\frac{b}{a}\right) \frac{\varepsilon-1}{2}\left(T_1 \cos\varphi\, \vec{i}_\varphi + T_2 \sin\varphi\, \vec{i}_\theta\right),$$

$$\vec{E}^{(1)}_{\mathrm{TM}}(\varphi,\theta) = \frac{\exp \mathrm{i}k_1 r}{k_1 r}\left(\frac{b}{a}\right) \left[\frac{\varepsilon-1}{2}T_3 \sin\varphi\, \vec{i}_\varphi + \left(\frac{\varepsilon-1}{2\varepsilon}T_4 + \frac{\varepsilon-1}{2}T_5\cos\varphi\right)\vec{i}_\theta\right], \tag{42}$$

where $\vec{i}_\varphi$, $\vec{i}_\theta$ are the unit vectors of the spherical coordinate system, and T_i are complex expressions including the angular spheroidal functions.

It is important that all the functions T_i do not depend on the dielectric permittivity of the particle ε. Therefore, comparing expressions (41)–(42) with those of the Rayleigh-Gans approximation (RGA; $|\varepsilon-1| \ll 1,\ c_1|\varepsilon-1| \ll 1$) we can find that

$$T_1 \equiv \frac{2c_1^3}{3}G(u), \quad T_2 \equiv \frac{2c_1^3}{3}\cos\theta\, G(u), \quad T_3 \equiv -\frac{2c_1^3}{3}\cos\alpha\, G(u),$$

$$T_4 \equiv \frac{2c_1^3}{3}\sin\alpha\, G(u), \quad T_5 \equiv \frac{2c_1^3}{3}\cos\alpha\cos\theta\, G(u). \tag{43}$$

Here the function

$$G(u) = \frac{3}{u^3}(\sin u - u\cos u), \tag{44}$$

where for a prolate spheroid

$$u = c_1|\cos\theta - \cos\alpha| \tag{45}$$

and for an oblate one

$$u = c_1\sqrt{\sin^2\alpha + \sin^2\theta - 2\sin\alpha\sin\theta\cos\varphi}. \tag{46}$$

Note that expressions (41)–(42) coincide with those of the Rayleigh approximation (RA; $c_1 \ll 1$, $c_1|\varepsilon| \ll 1$) if one excludes the factor $G(u)$. Since $G(0) = 1$, the RA is a particular case of the approximation provided by Eqs. (41)–(46). We call this generalization of the RA and RGA the quasistatic approximation [42].

The physical sense of the approximation is seen from the fact that actually we represented the field inside a particle by the incident field $\vec{E}^{(0)}$ (like in the RGA), taking into account the particle polarizability (like in the RA)

$$\vec{E}^{(2)} = \frac{\hat{\alpha}\,\vec{E}^{(0)}}{(\varepsilon-1)V} = K_x E_x^{(0)}\vec{i}_x + K_y E_y^{(0)}\vec{i}_y + K_z E_z^{(0)}\vec{i}_z, \tag{47}$$

where $\hat{\alpha}$ is the polarizability tensor, V the volume of a homogeneous particle, $(\vec{i}_x, \vec{i}_y, \vec{i}_z)$ are the unit vectors of the Cartesian system (x, y, z) connected with the particle axes, $K_{x,y,z} = ((\varepsilon-1)L_{x,y,z}+1)^{-1}$, and $L_{x,y,z}$ are the geometrical factors changing from 1/3 for a sphere to about 1 (0) for a particle very elongated (flattened) in the given direction, e.g.

$$L_x = abc\int_0^{\infty} \frac{\mathrm{d}q}{(a^2+q)f(q)}, \tag{48}$$

where a, b, c are the semiaxes of the ellipsoid and $f(q) = \sqrt{(a^2+q)(b^2+q)(c^2+q)}$ (see [43] for more details).

The RA is known for ellipsoids with confocal (coaxial) boundary layers (see, e.g. [43]). We extend it and the QSA for multilayered ellipsoids with *nonconfocal* boundaries of layers [27]. Use of the asymptotic of the mEBCMsc is possible here only for confocal boundaries, as for the nonconfocal ones the analytic expressions of the RGA and RA do not exist. Therefore, another way of solution based on Eq. (47) is utilized. Generally, the problem is to solve the Laplace equation with the corresponding boundary conditions. Because of the nonconfocality of boundaries, each layer of the particle is divided into a number of sublayers with its own ellipsoidal coordinate system defined inside. For any sublayer, approximate boundary conditions are formulated (see [44] for more details). As a result we obtain the following expression for the polarizability along the axis of the coordinate system connected with the particle:

$$\alpha_{x,y,z} = V\frac{\bar{\varepsilon}_{x,y,z}-1}{(\bar{\varepsilon}_{x,y,z}-1)L_{x,y,z}+1}, \tag{49}$$

where

$$\bar{\varepsilon}_{x,y,z} = B_2/B_1 \tag{50}$$

and for example, for the x-axis direction

$$\begin{pmatrix} B_1 \\ B_2 \end{pmatrix} = \begin{pmatrix} 1 & L_{x,n} \\ \varepsilon_n & \varepsilon_n(L_{x,n}-1) \end{pmatrix} \Psi \begin{pmatrix} (\varepsilon_1-1)L_{x,1}+1 \\ -(\varepsilon_1-1)\delta_1 \end{pmatrix}. \tag{51}$$

Here $\varepsilon_j = \varepsilon_j/\varepsilon_{j+1}$, and ε_j, $L_{x,j}$, δ_j are the permittivity in the jth layer, the geometrical factor and the fraction of volume related to its external boundary, respectively, and

$$\Psi = \prod_{j=2}^{n-1}(\Omega_j\Gamma_j)\Omega_1, \quad \Omega_j = C_j\prod_{l=1}^{n_{\mathrm{sub}}}\Lambda_{jl}, \tag{52}$$

where C_j are some constants, the 2×2 matrices Ω_j and Γ_j depend only on the parameters of the jth layer $(\varepsilon_j, L_j, \delta_j)$, and the 2×2 matrices Λ_{jl} depend only on these parameters for the lth sublayer of the jth layer [44]. In the case of the confocal boundaries of layers one has $\Lambda_{jl} = \Omega_j = I$ and for

$j = 2, 3, \ldots, n-1$

$$\Gamma_j = \begin{pmatrix} (\varepsilon_j - 1)L_{x,j} + 1 & \dfrac{(\varepsilon_j - 1)}{\varepsilon_j} L_{x,j}(L_{x,j} - 1) \\ -(\varepsilon_j - 1)\delta_j & -(\varepsilon_j - 1)(L_{x,j} - 1) + 1 \end{pmatrix}. \tag{53}$$

In principle Eq. (51) can be rewritten in the recursive form (see [42] for more details).

Note that the quantity $\bar{\varepsilon}$ appearing in the formulation of the QSA and RA for layered scatterers (see Eq. (50)) can be interpreted as an averaged dielectric permittivity. For small particles ($|m-1|x_V < 1$, where the size parameter $x_V = 2\pi r_V/\lambda$, r_V is the radius of sphere whose volume is equal to that of the spheroid, λ the wavelength of incident radiation), it was used to produce a new mixing rule of the effective medium theory (EMT). This rule takes into account the internal structure of particles and as our calculations demonstrate, gives for layered ellipsoids significantly more accurate results than other mixing rules (see Section 7.3).

7. Applicability of the methods

Here we analyze the applicability ranges of the exact methods suggested and compare the theoretical conclusions with the results of numerical experiments. Comparison of our computer programs with those realizing other methods is made when possible. The codes are also used to discuss applicability of the approximate methods considered in Section 6.

7.1. Exact methods: analytic investigation

Both exact methods (mEBCM and mEBCMsc) extended by us to layered particles are modifications of the EBCM. Therefore, analytic consideration of their applicability ranges can be based on the analysis of EBCM-like methods made for homogeneous particles in [23]. Below we first briefly describe the main results of that analysis and then consider the differences appearing for layered scatterers.

It is well known that singularity of the systems of algebraic equations for the coefficients of expansions of the fields or potentials is the main reason of limited applicability of the EBCM for high eccentricity scatterers (see, e.g. [2]). To large extent this singularity is a consequence of divergence of these expansions. For homogeneous particles, the infinite systems for the expansion coefficients of the internal ($\vec{a}^{(2)}$) and scattered ($\vec{a}^{(1)}$) field potentials look as follows (cf. Eqs. (16), (30)):

$$A_1\vec{a}^{(2)} = \vec{a}^{(0)}, \quad \tilde{A}_1\vec{a}^{(1)} = \tilde{A}_2\vec{a}^{(0)}. \tag{54}$$

Here $\tilde{A}_1, \tilde{A}_2$ are some matrices, $\tilde{A}_2\tilde{A}_1^{-1} = A_2A_1^{-1}$, where A_1, A_2 are from Eqs. (16), (30). The standard EBCM is mathematically correct (the expansions of the internal and scattered fields converge up to the scatterer boundary, i.e. the Rayleigh hypothesis is satisfied) under two conditions (see, e.g. [19,23]):

1. All peculiarities of the analytic continuation of the scattered field lie inside the maximum sphere inscribing the particle (we denote its radius by $r_{\rm in}$).

2. All peculiarities of the analytic continuation of the internal field lie outside the minimum sphere circumscribing the particle (the radius $r_{\rm out} > r_{\rm in}$).

These conditions can be written as follows:

$$d_{\rm sca} < r_{\rm in}, \quad r_{\rm out} < d_{\rm int}, \tag{55}$$

where $d_{\rm sca}$ and $d_{\rm int}$ are the distances from the coordinate origin to the closest and farthest peculiarities of analytic continuations of the scattered and internal fields, respectively. Note that these conditions are not applicable to the discrete source method (as a modification of the EBCM) and nonstandard (i.e. different from used by P.Waterman, P.Barber et al.—see [2]) EBCM versions, where a non-free-space Green's function is used (e.g. [34]) or the expansion coefficients of the scattered field are determined in a least-squares sense (see [19] for more details). In the last case the expansion converges uniformly everywhere outside the scatterer, but finding the expansion coefficients presents a special problem [19].

The situation is different when one considers the optical properties of scatterers only in the far zone, i.e. cross-section, phase function, etc. In this case an integro-operator equation connecting the field at the surface of a scatterer with the far-field pattern can be written (see [22,23]). In this equation for the pattern one can substitute its expansion in terms of the angular spherical wave functions and use the Sommerfeld integrals [45] to represent the spherical Hankel functions of the first kind. Taking into account the orthogonality of the angular spherical wave functions on any sphere with the center at the coordinate origin, an algebraic system for the coefficients of the pattern expansion can be obtained (see [22] for more details). It is important that as a result one gets the same system as for the basically used version of the EBCM [23]. In other words, two ways to find the scattered field in the far zone (by solution of the equation for the pattern and usual EBCM equations) are equivalent, and hence their applicability ranges must be the same. As the equation for the pattern does not require convergence of the expansions up to the scatterer boundary we can conclude that validity of the Rayleigh hypothesis is not necessary for consideration of the optical characteristics in the far zone in the EBCM, and only the condition of solvability of the systems should be satisfied. This condition was found by analyzing the behavior of the matrix elements of the systems in the large index value regions in [22,23]. We used the asymptotics of the spherical Bessel and Hankel and associated Legendre functions for large indices, the saddle point approximation to evaluate the integrals in the matrix elements (the parameter θ was made complex) [18], and the renormalization of unknowns and free terms

$$x_n^{(1)} = \frac{2^n n!}{(k_1 R)^n} a_n^{(1)}, \quad x_l^{(0)} = \frac{(k_2 R)^l}{2^l l!} \tilde{a}_l^{(0)}, \tag{56}$$

where R is a free parameter, and $\vec{\tilde{a}}^{(0)} = \tilde{A}_2 \vec{a}^{(0)}$. For the axisymmetric part, we arrived to the system (see [23] for more details)

$$\sum_{n=1}^{\infty} \tilde{\alpha}_{ln}^{(1)} \, x_n^{(1)} = x_l^{(0)}, \quad l = 1, 2, \ldots \tag{57}$$

with the following constraints:

$$|\tilde{\alpha}_{ln}^{(1)}| \leqslant \text{Const}\left(\frac{1}{l}\right)\left(\frac{d_{\rm sca}}{R}\right)^l \left[1 + \text{O}\left(\frac{1}{l}\right)\right], \quad l \gg 1, \; n = \text{O}(1), \tag{58}$$

$$|\tilde{\alpha}_{ln}^{(1)}| \leqslant \mathrm{Const}\left(\frac{R}{d_{\mathrm{int}}}\right)^{n}\left[1+\mathrm{O}\left(\frac{1}{n}\right)\right], \quad n \geqslant l, \tag{59}$$

$$\tilde{\alpha}_{ll}^{(1)} = \frac{1}{2}\left(1+\frac{k_1}{k_2}\right)\left[1+\mathrm{O}\left(\frac{1}{l}\right)\right], \quad \tilde{\alpha}_{ln}^{(1)} = \mathrm{O}\left(\frac{1}{ln}\right), \quad l, n \geqslant 1, \; |n-l| = \mathrm{O}(1), \tag{60}$$

$$|x_l^{(0)}| \leqslant \mathrm{Const}\frac{1}{l}\left(\frac{d_{\mathrm{in}}}{R}\right)^{l}\left[1+\mathrm{O}\left(\frac{1}{l}\right)\right], \quad l \geqslant 1, \tag{61}$$

where

$$d_{\mathrm{sca}} = \max|r(\theta_0)\mathrm{e}^{\mathrm{i}s\theta_0}|, \tag{62}$$

$$d_{\mathrm{int}} = \min\left|r(\theta_0)\mathrm{e}^{\mathrm{i}s\theta_0}\right| \tag{63}$$

and values of θ_0 are found from the equations

$$\left.\frac{r'_\theta(\theta)}{r(\theta)}\right|_{\theta=\theta_0} = -\mathrm{i}s, \tag{64}$$

$$\exp\,(\mathrm{i}s\,\theta_0) = 0 \tag{65}$$

with $s = 1$ or -1. It should be mentioned that besides the roots of these equations one should also consider all nonanalytic points of the scatterer surface. The system (57) with the constraints (58)–(61) is quasiregular [24,36,46] and the Fredholm alternative is valid for it under the condition

$$\max(d_{\mathrm{in}}, d_{\mathrm{sca}}) \leqslant R \leqslant d_{\mathrm{int}}. \tag{66}$$

Note that there are no peculiarities for a plane incident wave, i.e. $d_{\mathrm{in}} = 0$. Taking into account the uniqueness of the solution of the scattering problem, we conclude that when (66) is valid, there must be the only solution of the systems (57) which can be found by the reduction method [24,36,46]. The last point is of particular importance since in numerical calculations one always solves truncated systems.

For the nonaxisymmetric parts, we get the system with the constraints analogous to (58)–(61). In [23] it was also shown that a similar analysis could be applied to any version of the EBCM, involving (nonmultipole) expansions of the fields or potentials in terms of the (spherical) wave functions and formulation of the problem as surface integral equations. Thus, the necessary condition of applicability of the EBCM in the far zone can be formulated in such a way [23]:

3. All peculiarities of the analytic continuation of the divergent fields (i.e. those corresponding to the potentials with the subscript 2 in our EBCM modification $-p_2$, U_2, etc.) lie farther from the coordinate origin than all peculiarities of analytic continuation of the convergent fields (i.e. those corresponding to the potentials with the subscript 1 $-p_1$, U_1, etc.).

In the used notations (for a plane incident wave) it just means

$$d_{\mathrm{sca}} < d_{\mathrm{int}} \tag{67}$$

and one can easily see that Eq. (67) puts less tight constraints on the particle geometry than Eq. (55) as always $r_{\rm in} < r_{\rm out}$. Positions of the peculiarities in the cases of spheroidal and Chebyshev particles, i.e. expressions for $d_{\rm sca}$ and $d_{\rm int}$, and comparison with results of numerical calculations can be found in [23].

It should be added that the results obtained for homogeneous particles in [23] are consistent with those of other authors. The paper [23] extends the works of Kyurkchan (see [22] and references therein) and hence agrees with all his results including the condition (67) suggested first in [22] for perfectly conducting scatterers. The condition of convergence of the series in the EBCM for the far zone found in [21] is too complicated to be applied to Chebyshev particles, but for spheroids it is valid (see the proof in [21]) as well as the condition (67) [22,23].

Let us now expand the analysis to layered particles and start with the Rayleigh hypothesis. Obviously for cores of layered particles we have the standard conditions

$$d_{\rm sca}^{(n)} < r_{\rm in}^{(n)}, \quad r_{\rm out}^{(n)} < d_{\rm int}^{(n)}. \tag{68}$$

However, for other layers, the situation is a bit different and the conditions can be formulated as follows:

1′. All peculiarities of the analytic continuations of the divergent fields lie inside a maximum sphere inscribing the inner surface of the layer.
2′. All peculiarities of the analytic continuations of the converging fields lie outside a minimum sphere circumscribing the outer surface of the layer.

As a result we have

$$d_{\rm sca}^{(j)} < \; r_{\rm in}^{(j+1)}, \quad r_{\rm out}^{(j)} < \; d_{\rm int}^{(j)}, \; j = 1, 2, \ldots, n-1, \tag{69}$$

where the superscript j denotes the quantities related to the surface S_j. As $r_{\rm in}^{(j+1)} < r_{\rm in}^{(j)}$, the conditions (69) are always more strong than the conditions (55) for the same surface S_j. Obviously, conditions (55) and (69) coincide for an extremely thin layer ($r^{j+1} \to r^j$).

For layered particles, the solvability conditions (66) must be satisfied for all layer boundaries and the parameter R must be kept the same as Eqs. (16) and (17) for the boundaries are coupled. In other words, the expansions of the potentials for all layers should converge in a common spherical ring. It takes place provided:

3′. All peculiarities of the analytic continuation of the divergent fields in all layers lie farther from the particle center than all peculiarities of the analytic continuation of the convergent fields in all layers.

It means that

$$\max\{d_{\rm sca}^{(j)}\}_{j=1}^{n} < \; \min\{d_{\rm int}^{(j)}\}_{j=1}^{n}. \tag{70}$$

For confocal spheroids, $d_{\rm sca}^{(j)} = d/2$ for all j and Eq. (69) automatically lead to the inequality (70) as $d_{\rm sca}^{(j)} < r_{\rm in}^{(n)} < r_{\rm out}^{(n)} < r_{\rm out}^{(j)} < d_{\rm int}^{(j)}$ for any j.

Our analysis shows that the condition $3'$ is the only one required for calculations in the far zone. For homogeneous particles, condition (70) is equivalent to Eq. (67), and condition $3'$ was not added to conditions 1 and 2 as it automatically followed from them.

Thus, our modification of the EBCM is mathematically correct for particles with the layer boundaries satisfying the conditions formulated for the homogeneous scatterers (55) and supplemented with additional constraints. One of them connects the position of peculiarities defined by the external boundary of the layer with the parameters of its internal boundary (see the first inequality in Eq. (69)). Another additional condition, which is also the only one necessary for the far zone, is an intersection of conditions (67) for homogeneous particles applied to each layer boundary. Note that these conditions are valid for any modification of the EBCM where fields (or potentials) are expanded in terms of the spherical wave functions and the expansions are substituted in surface integral equations with the free-space Green's function.

Easy to see that all the conditions formulated above for the EBCM are in principle applicable to the EBCM in spheroidal coordinates for both homogeneous and layered spheroidal particles. The only difference of the methods, which is important here, is that the fields (potentials) are expanded in terms of the spheroidal wave functions instead of the spherical ones, and hence in the conditions one should replace spheres by spheroids and radius by the spheroidal coordinate ξ, to measure the distances in the curvilinear coordinate system, etc. It should be also noted that the peculiarities of the scattered field for prolate homogeneous spheroids are known to be in the foci and for oblate ones on the focal circle perpendicular to the particle symmetry axis, i.e. in both cases lie inside a spheroid, whereas the peculiarities of the internal field are located outside the scattering particle [23]. Therefore, for homogeneous spheroids conditions (55) and (67) are always satisfied. For a spheroid with the confocal boundaries of layers, conditions (68)–(70) are always valid as well. In other words the EBCM in spheroidal coordinates is mathematically correct for *any* homogeneous and layered spheroids with the confocal boundaries. Note that the analytic study of our SVM modification made in [24] has demonstrated that it is applicable to homogeneous spheroids of any shape and calculations have shown that even its efficiency does not depend on the aspect ratio a/b in contrast with the standard SVM (see [30] for more details).

7.2. Exact methods: numerical consideration

We have created computer programs realizing both theoretical methods suggested for layered particles (gmEBCM and gmEBCMsc). The codes were tested in the ways described, e.g., in [47]. Comparison with the codes available for multilayered spheres [48] and confocal core-mantle spheroids [5] as well as the DDA code [49] slightly modified to treat multilayered particles has demonstrated correctness of our programs in all considered cases. Improvement of the code based on the EBCM in spheroidal coordinates (gmEBCMsc) is in progress and below we shall discuss in more detail the program realizing the gmEBCM.

Convergence of the solutions is illustrated by Figs. 1–3, which also show accuracy that can be expected for three-layered spheroids treated by the gmEBCM (about 6 digits) and gmEBCMsc (about 13 digits).

The convergence behavior for the gmEBCM seen in the figures is typical of EBCM-like methods (see [23])—convergence occurs for the number of terms, being kept in solution, $N < 15$–25 (for double precision calculations), until the systems become ill-conditioned, and then (after some plato)

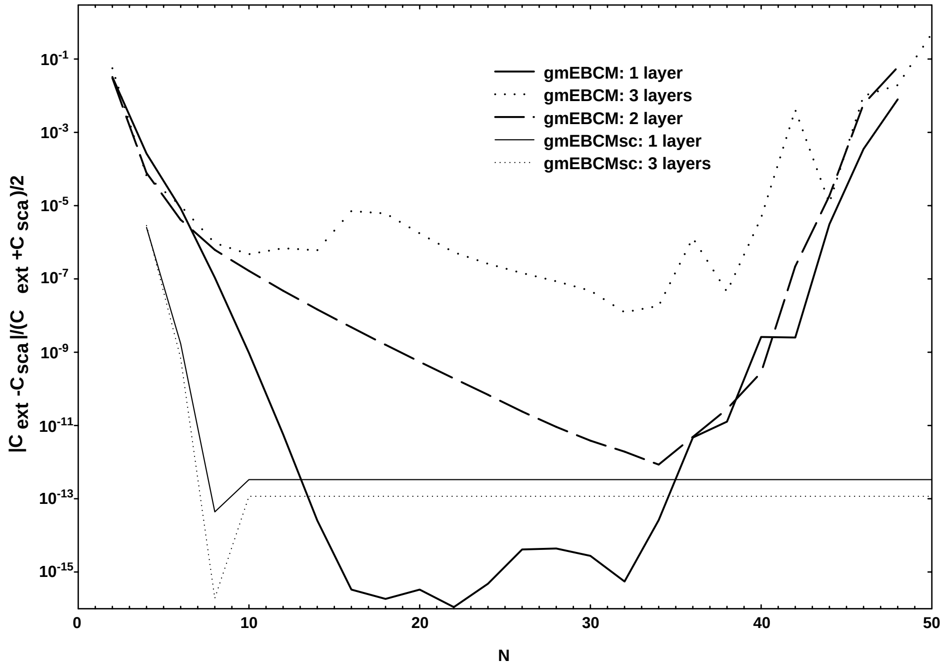

Fig. 1. Relative errors of energy conservation for dielectric spheroids. The refractive index and the volume fraction of core/layer/mantle of the three-layered spheroids are $(m, \delta_V) = (1.7, 0.34)/(1.0, 0.33)/(1.3, 0.33)$; the inclination angle $\alpha = 90°$, the size parameter $x_V = 2$; the aspect ratio of core/layer/mantle for the gmEBCM and that of core for the gmEBCMsc $a/b = 1.4$ (other ratios were derived from confocality condition (26)). For homogeneous spheroids, the refractive index of all layers is $m = \sqrt{\bar{\varepsilon}}$ with $\bar{\varepsilon}$ from Eq. (50); for core-mantle spheroids, $m_l = m_c = 1.7$.

accuracy of results decreases with N. For the mEBCMsc (and earlier mSVM), we generally do not have singular systems and therefore the accuracy remains at the level of computational errors (about 10^{-14}–10^{-15}). This difference of the methods appears due to the absence of the radial functions getting very large/small values in the matrix elements (cf. Eqs. (30), (31) and (16)).

Figs. 2 and 3 illustrate convergence of the gmEBCM for three-layered spheroids of different aspect ratio a/b, refractive index m, and size parameter x_V. One can see that like for homogeneous particles (see [23]) convergence (here we mean the slope of curves for small N, where the convergence really occurs) practically does not depend on m and x_V and is affected only by a/b. This corresponds to general results of our theoretical analysis in previous subsection which predicted that the convergence should depend only on the shape of a scatterer. Note that the analysis was made for infinite systems, while in calculations we always deal with finite (truncated) systems whose properties for small N may be partly different. We should also add that accuracy of the gmEBCM results (the plato for spheroids with two and three different layers in Fig. 1) may be affected by inappropriate formulation of the boundary conditions as took place, e.g., for homogeneous perfectly conducting particles in [50].

Our calculations show that the gmEBCM code (and the method) allows one to treat axisymmetric particles with up to about 10 layers and the size parameter $x_V \lesssim 5$–7 in a wide region of the refractive index values. Certain problems are met for essentially elongated/flattened particles

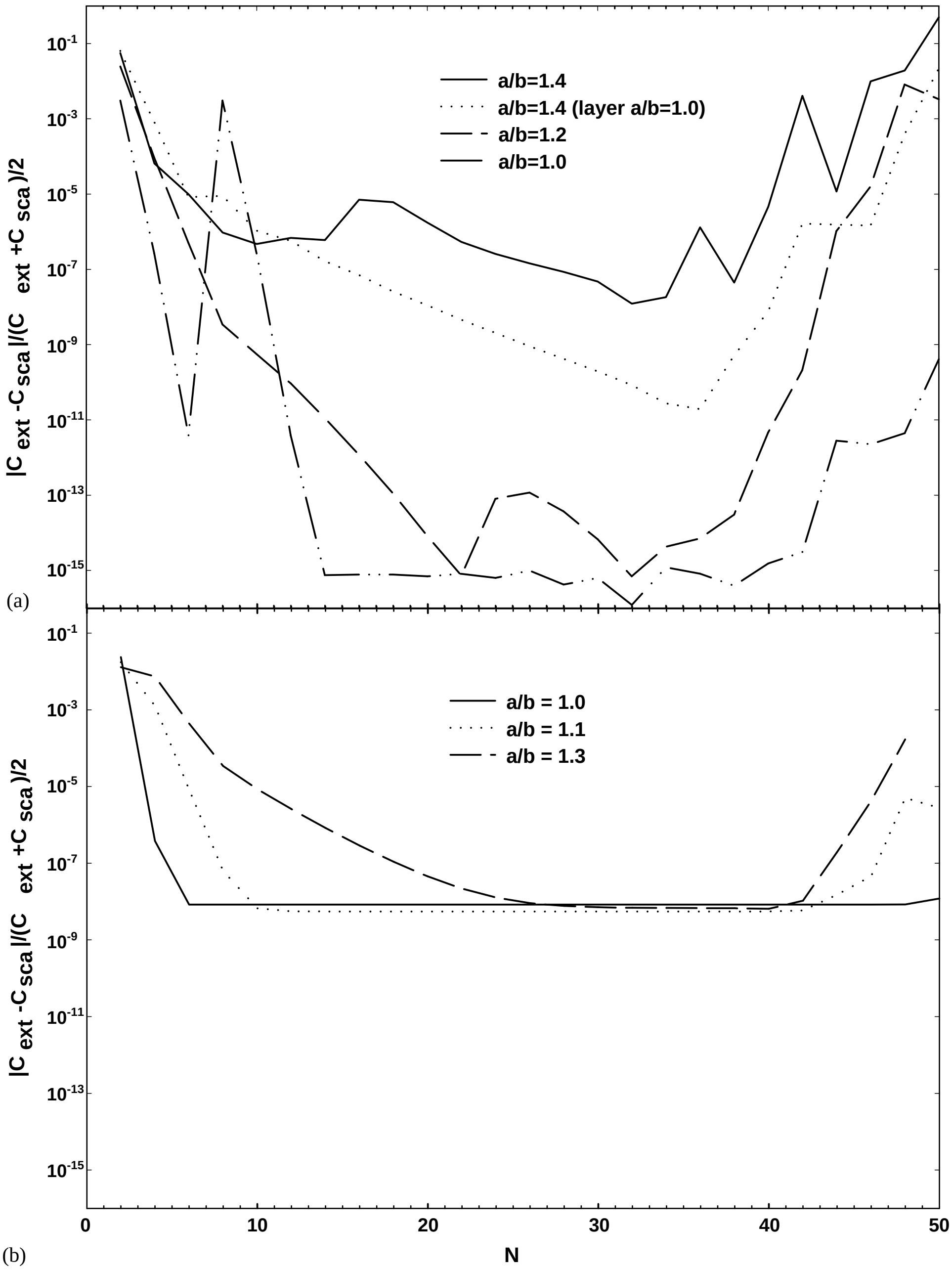

Fig. 2. Relative errors of energy conservation for three-layered dielectric spheroids of different aspect ratios a/b treated by the gmEBCM. The refractive indices and the volume fractions of core/layer/mantle and other parameters are as in Fig. 1. (a) $m_{\mathrm{m}} = 1.3$; (b) $m_{\mathrm{m}} = 3$.

(e.g., for spheroids for the aspect ratio $a/b > 2$). In this case, another method—the gmEBCMsc provides a solution applicable to multilayered spheroids with the confocal boundaries. The range of applicability of this solution is very large in a/b and x_{V} and needs a special study.

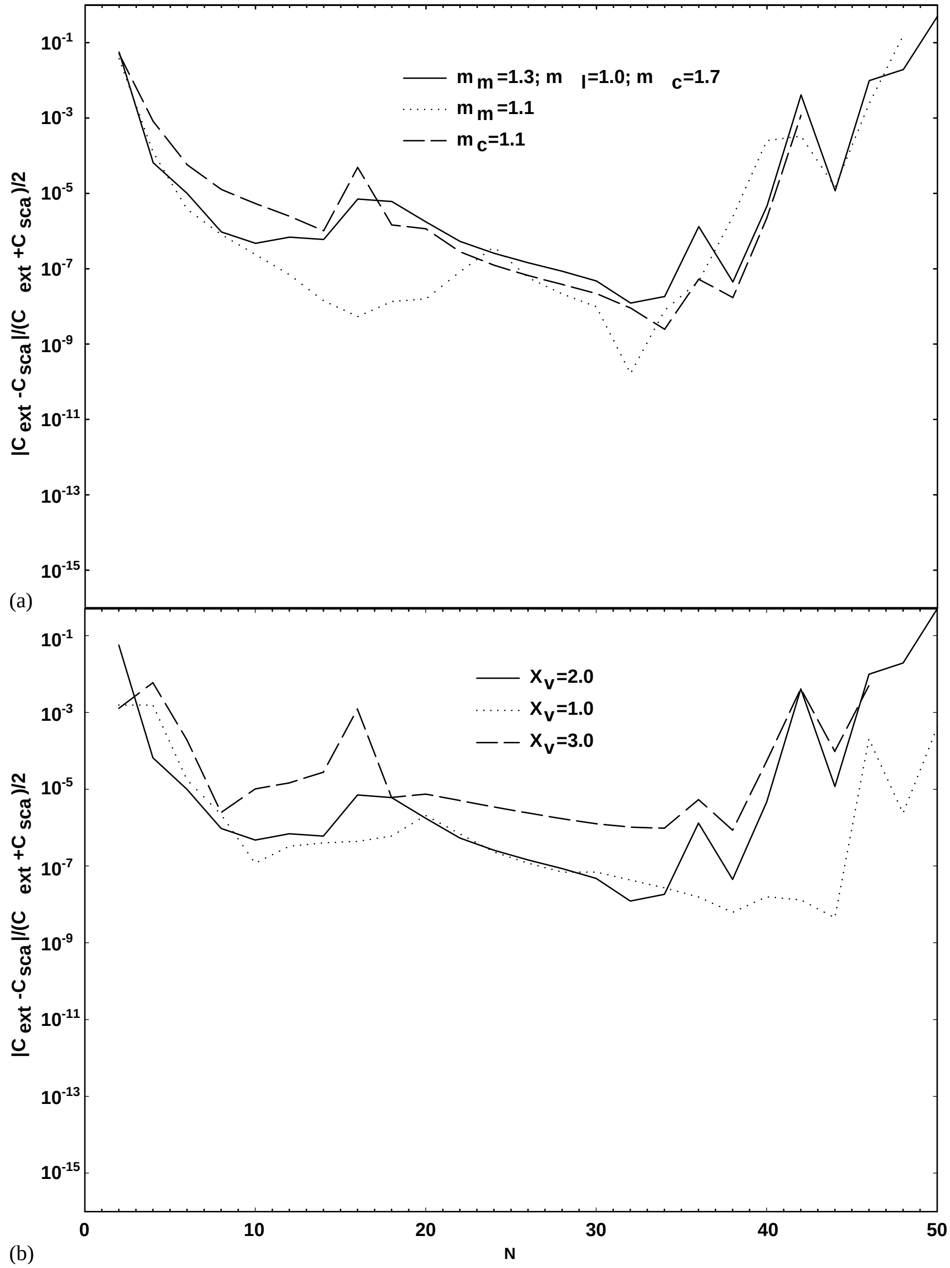

Fig. 3. Relative errors of energy conservation for three-layered dielectric spheroids of different refractive indices (a) and sizes (b) treated by the gmEBCM. The refractive indices (if not specified) and the volume fractions of core/layer/mantle and other parameters are as in Fig. 1.

Besides consideration of the applicability ranges, it is useful to compare the efficiency of the methods (codes) with the DDA [49], being a good representative of the universal volume integral equation methods. We find that our gmEBCM code having higher accuracy needs an order of magnitude less memory and computational time. For instance, for a three-layered particle with $x_V = 4$, the gmEBCM code requires 5 Mb and 0.5 min for a 500 MHz PC, while the DDA one does 100 Mb and 30 min. Computational time for the gmEBCM, t, grows with an increase of the scatterer size much slower than for the DDA. Although $t \propto n$, where n is the number of layers, for large n the number of dipoles in the DDA should be increased to reproduce correctly the scatterer structure and this enlarges computational time as well. The gmEBCMsc code, being many orders of magnitude more accurate, needs memory nearly as much as the gmEBCM one. Computational time for the gmEBCMsc is of the order of t and its dependence on parameters is generally similar to that of the gmEBCM. Thus, the codes created by us well supplement each other and among other wide applications provide a good possibility to study applicability of the approximate methods for layered particles.

7.3. Approximate methods

The well known general conditions of applicability of the RA ($x \ll 1, |m|x \ll 1$) and RGA ($|m-1| \ll 1, |m-1|x \ll 1$) are formulated for spheres with the size parameter $x = 2\pi r/\lambda$, where r is the radius. For nonspherical particles, the conditions should be rewritten, for example, for the RA as follows:

$$x_d \ll 1, \quad |m|x_d \ll 1, \tag{71}$$

where x_d is the size parameter related to the maximum dimension of the particle.

The procedure that we utilized to construct the QSA for homogeneous spheroids in Section 6 (via the asymptotic of the scattered field in the gmEBCMsc) shows that for nonspherical particles the condition of applicability of the QSA can be formulated as

$$|m-1|x_V \ll 1, \tag{72}$$

where x_V is the size parameter related to the radius of a sphere whose volume is equal to that of the nonspherical particle. The difference of the conditions (71) and (72) becomes essential for scatterers of large eccentricity. For spheroids, the ratio $x_V/x_d \propto (a/b)^\alpha$, where $\alpha = \frac{1}{3}$ or $\frac{2}{3}$, and, for instance, for prolate particles with the aspect ratio $a/b = 30$ and $x_V = 0.1$, the QSA may give good results, whereas the RA should not be applied as $x_d > 1$. Calculations in [26] well confirm this general conclusion.

Such a shape dependence of the applicability ranges of the QSA and RA takes place for layered particles as well, although the situation for them becomes a bit more complicated. Not all layers of such particles give comparable contributions to the process of scattering, and nearly always there is a main layer. Our experience indicates that, to a first approximation, it can be identified as a layer with the maximum product $|m-1|V$, where m and V are the refractive index and the volume of the layer. It is the shape of the outer boundary of the main layer which is important for the QSA efficiency. If the eccentricity of this boundary is intermediate or large (the ratio of the maximum to minimum dimensions exceeds 2–3), the QSA is always preferable to the RA. The inner boundary of the main layer also plays a role. It is less important simply because typically its surface area is essentially smaller than that of the outer boundary. An empirical factor characterizing the relative importance of the QSA over the RA could look as follows: $l^{\rm o}_{\max}/l^{\rm o}_{\min} + V^{\rm i}/V^{\rm o} l^{\rm i}_{\max}/l^{\rm i}_{\min}$, where $l_{\max}$ and $l_{\min}$ are the maximum and minimum dimensions of a

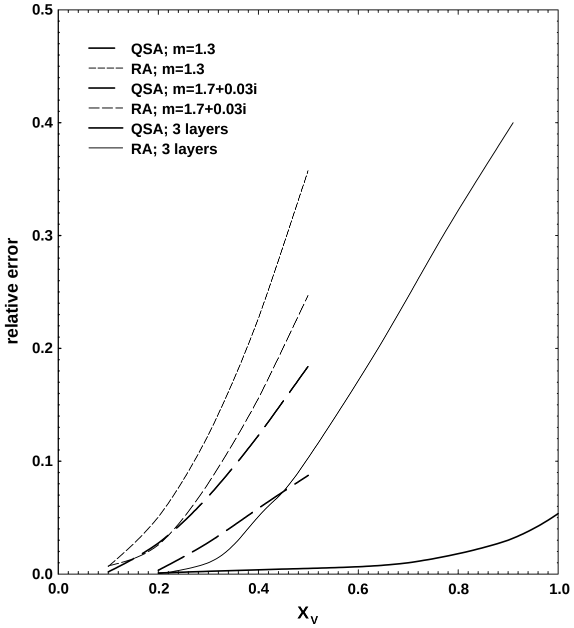

Fig. 4. Relative errors of the scattering cross-sections derived with the RA and QSA for homogeneous ellipsoids with the semiaxis ratio $a:b:c=$ 6.5:3:1 and the refractive indices $m = 1.3$ and $1.7 + 0.03i$ as well as for three-layered ellipsoids with the semiaxis ratios, refractive indices and volume fractions of core/layer/mantle $(a:b:c, m, \delta_v) = (4:2:1, 1.3+0i, 0.22)/(6.5:3:1, 1.7+0.03i, 0.34)/(20:7:1, 1+0i, 0.44)$; $\alpha = 90^\circ$.

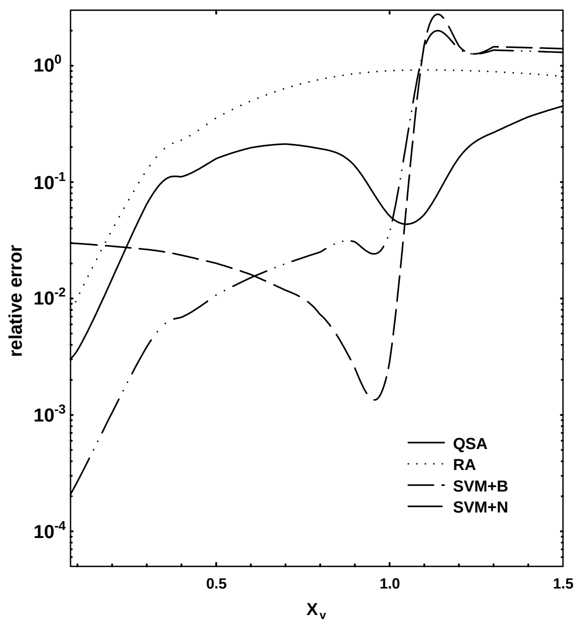

Fig. 5. Relative errors of the scattering cross-sections calculated with a SVM code for homogeneous particles with the permittivity according to the new EMT rule (SVM+N; dash-dot-dot curve) in the case of two-layered confocal spheroids (mantle: $a/b = 4:1, m = 1.33 + 0.01i$; core: $a/b = 6.7:1, m = 1.7 + 0.03i$; the volume fraction of the core is 0.5). Results obtained with the standard Bruggeman rule of the EMT are denoted by SVM+B (dashed curve).

surface, and the superscripts o and i are related to the outer and inner boundaries of a layer, respectively.

An example of importance of the inner boundary is provided by the three-layered ellipsoids examined in Fig. 4. Due to the largest contribution to the volume-averaged refractive index the main layer of this particle is the middle one. Its outer boundary has the semiaxis ratio equal to that of the homogeneous ellipsoid also presented in the figure, but the difference between the RA and QSA for the ellipsoids is very large. We believe that it is the effect of significant eccentricity of the inner boundary of the main layer of the three-layered ellipsoid (and a relatively large ratio $V^{\mathrm{i}}/V^{\mathrm{o}}$).

We have compared the QSA with the most popular approximation—the RA and now discuss its comparison with some other approaches. Our program realizations of the EBCM (gmEBCM) and SVM (gmEBCMsc) show that due to relative complexity of the algorithms the size of codes and speed of calculations are at least an order of magnitude larger than those for the QSA in the nonconfocal case, which is not analytic and hence much more complicated. Also the restrictions of the EBCM and SVM should be noted. As far as we know there is no formulation of the SVM in ellipsoidal coordinates, i.e. this method is still mainly limited by spheroids with confocal boundaries (a generalized SVM suggested in [31] can be applied to scatterers of any shapes but its computational efficiency and applicability range are not clear). The efficiency of the EBCM for nonaxisymmetric particles is even lower than that of the DDA [51].

In principle most volume integral equation methods (e.g., the DDA) can be applied to multilayered ellipsoids. Our calculations performed with the DDA code [49] can serve as a test of these approaches. We found that this code required computational time that was orders of magnitude larger than that of the QSA in the nonconfocal case and accuracy of the DDA results were generally not much higher than the QSA ones. Note also that the QSA does not have strong demands to computer memory typical of the DDA.

It should be pointed out that the formulation of the QSA for layered particles with the confocal boundaries (see Eqs. (41)–(53)) does not contain any signs of the specific character (confocality) of these particles. We applied these formulas to particles with nonconfocal boundaries and found that such an approximation, being analytic and hence quite fast, was practically as accurate as the QSA formulated for nonconfocal boundaries.

Now we turn to the EMT which is used to replace long (or even impossible) calculations of the optical properties of inhomogeneous particles by calculations for homogeneous ones with an averaged refractive index (see, e.g. [43]). We compared the rule provided by Eqs. (50)–(53) with the standard ones for layered spheroids (for multilayered spheres it was done in [48]). It is found that in the region of small diffraction parameter values ($x_V < 0.3$), the new rule provides a very good approximation, in contrast to other rules of the EMT (cf. curves marked by SVM+N and SVM+B in Fig. 5). Note that the standard rules of the EMT, like the Bruggeman one used in Fig. 5, give a wrong limit at $x_V \to 0$, since, unlike the rule (57), they do not involve information on the internal structure of the scatterer.

8. Conclusions

We have further developed and systematically discussed several exact and approximate methods extended to treat light scattering by layered nonspherical particles. Comparative consideration of the methods allowed us to summarize their differences and connections.

Analytic and preliminary numerical investigations of the ranges of applicability of the methods (and codes) show their supplementary nature which can be useful in applications. The extended boundary condition method formulated in spheroidal coordinates and the analytic formulas of the quasistatic approximation were found to be in particular perspective for treatment of light scattering by multilayered nonspherical particles.

Acknowledgements

The authors thank anonymous referees for their comments essentially improved the manuscript, N.V.Voshchinnikov for useful discussions, and A.B.Zinov'ev for work on the gmEBCMsc code. V.I. acknowledges the support by the grant 00-15-96607 and Astronomy program of the Russian federal government. The work was partly supported by the INTAS grant 99/652.

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