CALCULATION FORMULAS FOR THE METHOD OF PERTURBATION OF THE MIE SCATTERER SHAPE ON THE BASIS OF VECTOR SPHERICAL HARMONICS ACCORDING TO THE ANGULAR MOMENTUM QUANTUM THEORY

D.N. Romashov, V.A. Yachmenev, and R.F. Rakhimov

Institute of Atmospheric Optics,
Siberian Branch of the Russian Academy of Sciences, Tomsk
Received October 12, 1994

Numerical realization is presented of the perturbation method of the Mie scatterer shape for arbitrary oriented perturbed sphere. The conversion is performed from the basis of vector spherical harmonics with real dependence on azimuth angle φ, conventional in the light scattering theory, to the basis with complex dependence on the angle φ. The convergence of the method is examined for different number of corrections to be considered. The scattering phase matrix elements are calculated for elongated and inverted spheroids.

1. INTRODUCTION

Possible practical applications of modern achievements of the theory of light scattering by nonspherical particles are far behind the requirements of applied science including atmospheric aerosol optics. An attempt to generalize the Mie theory for arbitrary shaped particles was undertaken in Ref. 1, where only the first-order approximation in the perturbation parameter was considered. Then Erma[2–4] derived the recursion formulas for the corrections to the Mie coefficients of any order and presented the final formulas only for fixed orientation of a scatterer.

Unfortunately, in the aforementioned papers the universal technique for numerical calculations of arbitrarily perturbed spherical scatterer, depending not only on the polar angle θ, but also on the azimuth angle φ is lacking. The calculation formulas presented in this paper eliminate this disadvantage due to conversion from the basis of two linearly polarized states (LP–representation) to the basis of clockwise and counterclockwise polarized states (CP–representation). As a result, electromagnetic fields are expanded into series in terms of the vector spherical harmonics according to the angular momentum quantum theory.[5] Calculations performed for a sphere with $r = a$ perturbed to a sphere with $r = a(1 + \varepsilon)$ show that in order to obtain reasonable accuracy of estimation of the light scattering parameters, it is necessary to consider the corrections of rather high order.

At the same time the development of the method of perturbation of the Mie scatterer shape (PMSS) is promising due to a number of its advantages over the other nonperturbation methods. In particular, the well–known Barber-Yeh method[6] proceeds from the equivalent statement of the problem of light scattering by arbitrarily shaped particle in the form of the vector integral equation. The problem is reduced to solving the infinite system of linear algebraic equations with infinite number of variables. The coefficients of equations are the integrals of the spherical functions with weights varying over the complex surface of a scatterer that are difficult for calculating. Integration in the PMSS method is made analytically over the full solid angle, i.e., over the unit sphere, with four integrals for each next correction. The only disadvantage of the PMSS method is its applicability only for moderately nonspherical particles; however, it offers advantage over the Asano–Yamamoto method,[7] which can be used only for spheroids.

The facts that the majority of natural light scattering particles are rather compact formations with low degree of nonsphericity and that the modern possibilities of optical measurements are such that their interpretation in the context of the Mie theory is not sufficiently advanced are decisive arguments in support of the further development of the PMSS method. It seems unexpedient and excessive to us to apply a method more cumbersome than PMSS for moderately nonspherical particles because it adds complexity to the Mie theory.

2. CALCULATIONAL TECHNIQUE

In this paper we consider scatterers whose surface is a sphere perturbed by the small parameter ε in the form of expression

$$r = a(1 + \varepsilon f(\theta, \varphi, \theta_0, \varphi_0, \psi_0)) , \qquad (1)$$

where a is the radius of a nonperturbed sphere; $f(\theta, \varphi, \theta_0, \varphi_0, \psi_0)$ is the function that determines the shape and orientation of perturbation; θ_0, φ_0, and ψ_0 are the Euler angles; and, r, θ, and φ are the spherical coordinates. It should be noted that Eq. (1) compares favourably with the Erma representation of the scatterer shape.[4] It considers any orientation of particles in relation to the incident radiation.

Analytical realization of the PMSS method supposes, as the Mie theory, a solution of the boundary problem of finding the complex vector field $\mathbf{E}^s$ in the region external to the closed surface S that would satisfy the Helmholtz vector equation

$$\nabla \times (\nabla \times \mathbf{E}) = k_1^2 \mathbf{E} , \qquad (2)$$

and the vector field $\mathbf{E}^2$ in the internal region that would satisfy the equation

$$\nabla \times (\nabla \times \mathbf{E}) = k_2^2 \mathbf{E} , \qquad (3)$$

with the boundary conditions

$$(\mathbf{E}^i + \mathbf{E}^s - \mathbf{E}^2) \times \mathbf{N} = 0, \qquad (4)$$

$$(\mathbf{H}^{\mathrm{i}} + \mathbf{H}^{\mathrm{s}} - \mathbf{H}^{2}) \times \mathbf{N} = 0, \tag{5}$$

for the complex vector field $\mathbf{E}^{\mathrm{i}}$ in the external region specified on the surface S, where $\mathbf{N}$ is the normal to S,

$$\mathbf{N} = r_{\mathrm{s}} \,/\, a\, \mathbf{C}(r - r_{\mathrm{s}})\big|_{r = r_{\mathrm{s}}} = (1 + f\,\varepsilon)\,\mathbf{e}_{\mathrm{r}} - \boldsymbol{\alpha}\,,\ \ \boldsymbol{\alpha} = \nabla_{\Omega} f. \tag{6}$$

Magnetic vector fields are expressed through the electric ones as follows:

$$\mathbf{H}^{\mathrm{i}} = k_1\, \nabla \times \mathbf{E}^{\mathrm{i}} \,/\, i\,\omega\,\mu_1\,, \tag{7}$$

$$\mathbf{H}^{\mathrm{s}} = k_1\, \nabla \times \mathbf{E}^{\mathrm{s}} \,/\, i\,\omega\,\mu_1\,, \tag{8}$$

$$\mathbf{H}^{2} = k_2\, \nabla \times \mathbf{E}^{2} \,/\, i\,\omega\,\mu_2\,. \tag{9}$$

In addition to the complex amplitudes of the incident field $\mathbf{E}^{\mathrm{i}}$ and $\mathbf{H}^{\mathrm{i}}$ with cyclic frequency ω, wave numbers k_1 and k_2, and magnetic permeability μ_1 in surrounding medium and μ_2 inside a scatterer, the following parameters are used in this problem:

$$\chi_1 = k_1 \,/\, i\,\omega\,\mu_1\,,\ \chi_2 = k_2 \,/\, i\,\omega\,\mu_2\,,\ k = k_1 \,/\, k_2\,,\ \chi = \chi_1 \,/\, \chi_2\,,$$

$$\rho_{10} = k_1\, a,\ \ \rho_{20} = k_2\, a,\ \ \rho_1 = k_1\, r,\ \ \rho_2 = k_2\, r.$$

In order to solve Eqs. (2)–(9) and find the scattered field $\mathbf{E}^{\mathrm{s}}$, $\mathbf{H}^{\mathrm{s}}$, the expansion of the fields in terms of vector spherical harmonics and determination of the amplitudes of partial waves is used in the PMSS method, as in the Mie theory:

$$\mathbf{E}^{\mathrm{s}} = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} (a_{n\,m}\, \mathbf{M}^{1}_{n\,m} + b_{n\,m}\, \mathbf{N}^{1}_{n\,m})\,, \tag{10}$$

$$\mathbf{H}^{\mathrm{s}} = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \chi_1\, (a_{n\,m}\, \mathbf{N}^{1}_{n\,m} - b_{n\,m}\, \mathbf{M}^{1}_{n\,m})\,, \tag{11}$$

$$\mathbf{E}^{2} = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} (c_{n\,m}\, \mathbf{M}^{2}_{n\,m} + d_{n\,m}\, \mathbf{N}^{2}_{n\,m})\,, \tag{12}$$

$$\mathbf{H}^{2} = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \chi_2 (c_{n\,m}\, \mathbf{N}^{2}_{n\,m} - d_{n\,m}\, \mathbf{M}^{2}_{n\,m})\,. \tag{13}$$

Here the fields are expanded in terms of vector spherical harmonics of the form:

$$\mathbf{M}^{1}_{n\,m} = h^{(1)}_{n}(\rho_1)\, \mathbf{Y}^{(0)}_{n\,m}\,, \tag{14}$$

$$\mathbf{N}^{1}_{n\,m} = \frac{1}{\rho_1} \frac{d}{d\,\rho_1}\big[\rho_1\, h^{(1)}_{n}(\rho_1)\big]\mathbf{Y}^{(1)}_{n\,m} + \sqrt{n(n+1)}\, \frac{h^{(1)}_{n}(\rho_1)}{\rho_1}\, \mathbf{Y}^{(-1)}_{n\,m}, \tag{15}$$

$$\mathbf{M}^{2}_{n\,m} = j_n(\rho_2)\, \mathbf{Y}^{(0)}_{n\,m}\,, \tag{16}$$

$$\mathbf{N}^{2}_{n\,m} = \frac{1}{\rho_2} \frac{d}{d\,\rho_2}\big[\rho_2\, j_n(\rho_2)\big]\, \mathbf{Y}^{(1)}_{n\,m} + \sqrt{n(n+1)}\, \frac{j_n(\rho_2)}{\rho_2}\, \mathbf{Y}^{(-1)}_{n\,m}\,. \tag{17}$$

The vector spherical functions are determined by the well–known relationships[5]

$$\mathbf{Y}^{(0)}_{n\,m} = \frac{i}{\sqrt{n(n+1)}} \left(i\, \frac{m}{\sin\theta}\, Y_{n\,m}\, \mathbf{e}_{\theta} - \frac{d\,Y_{n\,m}}{d\,\theta}\, \mathbf{e}_{\varphi} \right), \tag{18}$$

$$\mathbf{Y}^{(1)}_{n\,m} = \frac{1}{\sqrt{n(n+1)}} \left(\frac{d\,Y_{n\,m}}{d\,\theta}\, \mathbf{e}_{\theta} + i\, \frac{m}{\sin\theta}\, Y_{n\,m}\, \mathbf{e}_{\varphi} \right), \tag{19}$$

$$\mathbf{Y}^{(-1)}_{n\,m} = Y_{n\,m}\, \mathbf{e}_r\,, \tag{20}$$

where

$$Y_{n\,m} = \mathrm{e}^{i\,m\,\varphi}\, P^{m}_{n}(\cos\theta) \sqrt{\frac{(2\,n+1)\,(n-m)!}{4\,\pi(n+m)!}}\,, \tag{21}$$

$j_n(\rho)$ and $h^{(1)}_{n}(\rho)$ are the Bessel and Hankel functions of the first kind, respectively, and $P^{m}_{n}(\cos\theta)$ are the associated Legendre polynomials.

The PMSS method supposes first of all the representation of the surface S determined by Eq. (1) in the spherical coordinates, and the expansion of the physical parameters determining the boundary conditions in the power series in terms of the perturbation parameter ε

$$a_{n\,m} = \sum_{p=0}^{\infty} \sum_{n=0}^{\infty} \sum_{m=-n}^{n} a^{p}_{n\,m}\, \varepsilon^{p},\quad b_{n\,m} = \sum_{p=0}^{\infty} \sum_{n=0}^{\infty} \sum_{m=-n}^{n} b^{p}_{n\,m}\, \varepsilon^{p}, \tag{22}$$

$$c_{n\,m} = \sum_{p=0}^{\infty} \sum_{n=0}^{\infty} \sum_{m=-n}^{n} c^{p}_{n\,m}\, \varepsilon^{p},\quad d_{n\,m} = \sum_{p=0}^{\infty} \sum_{n=0}^{\infty} \sum_{m=-n}^{n} d^{p}_{n\,m}\, \varepsilon^{p}. \tag{23}$$

Thus, the solution of the boundary problem reduces to finding the coefficients of expansion of four partial amplitudes a^{p}_{nm}, b^{p}_{nm}, c^{p}_{nm}, and d^{p}_{nm}.

Since the coefficients at zero power of ε are the coefficients of the Mie solution, the other terms of expansion in series are the corrections to the Mie coefficients of the corresponding order. Knowing them, it is possible to find the characteristics of the scattered field. They can be found upon substitution of expansions into the boundary conditions. The differential equations are considered in this derivation because the spherical functions satisfy them.

Combining the terms with the higher-order perturbation coefficients from infinite sequence of pairs of resulting boundary conditions (after setting the expressions at different powers of ε equal to zero) and integrating these equations considering the property of orthogonality, we obtain two linear algebraic systems. Solving them results in recursion relations for corrections to the Mie coefficients:

$$a^{p}_{n\,m} = \frac{1}{\Delta_1} \int_0^{2\pi} d\varphi \int_0^{\pi} (\alpha^{0}_{n}\, \mathbf{T}_p\, \mathbf{Y}^{(1)*}_{n\,m} - \alpha^{1}_{n}\, \mathbf{S}_p\, \mathbf{Y}^{(0)*}_{n\,m}) \sin\theta\, d\theta\,, \tag{24}$$

$$b^{p}_{n\,m} = \frac{1}{\Delta_2} \int_0^{2\pi} d\varphi \int_0^{\pi} (\alpha^{1}_{n}\, \mathbf{T}_p\, \mathbf{Y}^{(0)*}_{n\,m} - \alpha^{0}_{n}\, \mathbf{S}_p\, \mathbf{Y}^{(1)*}_{n\,m}) \sin\theta\, d\theta\,, \tag{25}$$

$$c^{p}_{n\,m} = \frac{1}{k\,\Delta_1} \int_0^{2\pi} d\varphi \int_0^{\pi} (\beta^{0}_{n}\, \mathbf{T}_p\, \mathbf{Y}^{(1)*}_{n\,m} - \chi\, \beta^{1}_{n}\, \mathbf{S}_p\, \mathbf{Y}^{(0)*}_{n\,m}) \sin\theta\, d\theta\,, \tag{26}$$

$$d^{p}_{n\,m} = \frac{1}{k\,\Delta_2} \int_0^{2\pi} d\varphi \int_0^{\pi} (\beta^{1}_{n}\, \mathbf{T}_p\, \mathbf{Y}^{(0)*}_{n\,m} + \chi\, \beta^{0}_{n}\, \mathbf{S}_p\, \mathbf{Y}^{(1)*}_{n\,m}) \sin\theta\, d\theta\,. \tag{27}$$

Let a plane clockwise or counterclockwise polarized wave be incident on a scatterer. Then the electric and magnetic fields of the incident light can be expanded into series in vector spherical harmonics[8] (the factor $\exp(-i\omega t)$ is omitted in the paper):

$$\mathbf{E}^{\mathrm{i}}_{\pm} = E_0 \sum_{n=0}^{\infty} i^{n} \sqrt{4\,\pi(2\,n+1)}\, \big(\mathbf{M}_{n\,\pm 1} \pm \mathbf{N}_{n\,\pm 1}\big)\,, \tag{28}$$

$$\mathbf{H}^{i}_{\pm} = \chi_1 E_0 \sum_{n=0}^{\infty} i^n \sqrt{4\pi(2n+1)} \left(\mathbf{N}_{n\pm 1} \pm \mathbf{M}_{n\pm 1}\right), \qquad (29)$$

where the plus sign corresponds to the clockwise polarization, and the minus sign corresponds to the counterclockwise polarization. Then the expressions for the operators T_p and S_p have the form:

$$\mathbf{S}_p = \sum_{n,m} \sum_{q=1}^{p} \left[F_q\left(Q^{q}_{0nm}\mathbf{Y}^{(0)}_{nm} + Q^{q}_{1nm}\mathbf{Y}^{(1)}_{nm}\right) + \alpha_q Q^{q}_{nm} Y_{nm}\right], (30)$$

$$\mathbf{T}_p = \sum_{n,m} \sum_{q=1}^{p} \left[F_q\left(R^{q}_{0nm}\mathbf{Y}^{(0)}_{nm} + R^{q}_{1nm}\mathbf{Y}^{(1)}_{nm}\right) + \alpha_q R^{q}_{nm} Y_{nm}\right], (31)$$

where

$$F_q = f^q / q!\,,\ \boldsymbol{\alpha}_q = \nabla_\Omega F^q = \boldsymbol{\alpha} f^{q-1}/(q-1)!\,,\ \boldsymbol{\alpha} = \nabla_\Omega f,$$

$$Q^{q}_{0nm} = k\, c^{p-q}_{nm}\, \alpha^{q}_{n}\, \rho^{q}_{20} - a^{p-q}_{nm}\, \beta^{q}_{n}\, \rho^{q}_{10},$$

$$Q^{q}_{1nm} = k\, d^{p-q}_{nm}\, \alpha^{q+1}_{n}\, \rho^{q}_{20} - b^{p-q}_{nm}\, \beta^{q+1}_{n}\, \rho^{q}_{10},$$

$$Q^{q}_{nm} = \rho_{10}\, (d^{p-q}_{nm}\, \eta^{q-1}_{n}\, \rho^{q-1}_{20} - b^{p-q}_{nm}\, \eta^{q-1}_{n}\, \rho^{q-1}_{10}) \sqrt{n(n+1)}\,,$$

$$R^{q}_{0nm} = -\, k\, d^{p-q}_{nm}\, \alpha^{q}_{n}\, \rho^{q}_{20} + \chi\, b^{p-q}_{nm}\, \beta^{q}_{n}\, \rho^{q}_{10},$$

$$R^{q}_{1nm} = k\, c^{p-q}_{nm}\, \alpha^{q+1}_{n}\, \rho^{q}_{20} - \chi\, a^{p-q}_{nm}\, \beta^{q+1}_{n}\, \rho^{q}_{10},$$

$$R^{q}_{nm} = \rho_{10}\, (c^{p-q}_{nm}\, \sigma^{q-1}_{n}\, \rho^{q-1}_{20} - \chi\, a^{p-q}_{nm}\, \eta^{q-1}_{n}\, \rho^{q-1}_{10}) \sqrt{n(n+1)}$$

for $q = 1, 2, \ldots, p-1$,

$$Q^{p}_{0n\pm 1} = k\, c^{0}_{n\pm 1}\, \alpha^{p}_{n}\, \rho^{p}_{20} - d^{0}_{n\pm 1}\, \beta^{p}_{n}\, \rho^{p}_{10} - G_n\, \gamma^{p}_{n}\, \rho^{p}_{10},$$

$$Q^{p}_{1n\pm 1} = k\, d^{0}_{n\pm 1}\, \alpha^{p+1}_{n}\, \rho^{p}_{20} - b^{0}_{n\pm 1}\, \beta^{p+1}_{n}\, \rho^{p}_{10} \mp G_n\, \gamma^{p+1}_{n}\, \rho^{p}_{10},$$

$$Q^{p}_{n\pm 1} = \rho_{10}\, (d^{o}_{n\pm 1}\, \sigma^{p-1}_{n}\, \rho^{p-1}_{20} - b^{0}_{n\pm 1}\, \eta^{p-1}_{n}\, \rho^{p-1}_{10}) \mp$$

$$\mp G_n\, \lambda^{p+1}_{n}\, \rho^{p}_{10} \sqrt{n(n+1)}\,,$$

$$R^{p}_{0n\pm 1} = -\, k\, d^{0}_{n\pm 1}\, \alpha^{p}_{n}\, \rho^{p}_{20} + \chi\, b^{0}_{n\pm 1}\, \beta^{p}_{n}\, \rho^{p}_{10} \pm \chi\, G_n\, \gamma^{p}_{n}\, \rho^{p}_{10},$$

$$R^{p}_{1n\pm 1} = k\, c^{0}_{n\pm 1}\, \alpha^{p+1}_{n}\, \rho^{p}_{20} - \chi\, a^{0}_{n\pm 1}\, \beta^{p+1}_{n}\, \rho^{p}_{10} - \chi\, G_n\, \gamma^{p+1}_{n}\, \rho^{p}_{10},$$

$$R^{p}_{n\pm 1} = \rho_{10}\, (c^{0}_{n\pm 1}\, \sigma^{p-1}_{n}\, \rho^{p-1}_{20} - \chi\, a^{0}_{n\pm 1}\, \eta^{p-1}_{n}\, \rho^{p-1}_{10} -$$

$$-\, \chi\, G_n\, \lambda^{p+1}_{n}\, \rho^{p}_{10}) \sqrt{n(n+1)}\,,$$

$$G_n = \sqrt{4\pi(2n+1)}\; i^n,$$

and

$$\alpha^{p}_{n} = \frac{d^p}{d\rho_2^p}\left[\rho_2\, j_n(\rho_2)\right]_{\rho_2=\rho_{20}},\quad \beta^{p}_{n} = \frac{d^p}{d\rho_1^p}\left[\rho_1\, h^{(1)}_n(\rho_1)\right]_{\rho_1=\rho_{10}}, \qquad (32)$$

$$\sigma^{p}_{n} = \frac{d^p}{d\rho_2^p}\left[\frac{j_n(\rho_2)}{\rho_2}\right]_{\rho_2=\rho_{20}},\quad \eta^{p}_{n} = \frac{d^p}{d r_1^p}\left[\frac{h^{(1)}_n(\rho_1)}{\rho_1}\right]_{\rho_1=\rho_{10}}, \qquad (33)$$

$$\gamma^{p}_{n} = \frac{d^p}{d\rho_1^p}\left[\rho_1\, j_n(\rho_1)\right]_{\rho_1=\rho_{10}},\quad \lambda^{p}_{n} = \frac{d^p}{d\rho_1^p}\left[\frac{j_n(\rho_1)}{\rho_1}\right]_{\rho_1=\rho_{10}}, \qquad (34)$$

$$\Delta_1 = (\chi\, \alpha^0_n \beta^1_n - \alpha^1_n \beta^0_n)\,, \qquad \Delta_2 = (\alpha^0_n \beta^1_n - \chi\, \alpha^1_n \beta^0_n)\,. \qquad (35)$$

Thus, it follows from Eqs. (24)–(31) that calculation of the corrections to the Mie coefficients reduces to calculation of integrals of the form:

$$I_1 = \int_0^{2\pi} d\varphi \int_0^{\pi} \Phi(\theta,\varphi)\, \mathbf{Y}^{(0)}_{nm}\, \mathbf{Y}^{(0)*}_{n'm'} \sin\theta\, d\theta\,, \qquad (36)$$

$$I_2 = \int_0^{2\pi} d\varphi \int_0^{\pi} \Phi(\theta,\varphi)\, \mathbf{Y}^{(1)}_{nm}\, \mathbf{Y}^{(0)*}_{n'm'} \sin\theta\, d\theta\,. \qquad (37)$$

Really, other kinds of integrals lose their significance because the identities take place

$$\mathbf{Y}^{(0)}_{nm}\, \mathbf{Y}^{(0)*}_{n'm'} = \mathbf{Y}^{(1)}_{nm}\, \mathbf{Y}^{(1)*}_{n'm'}\,, \qquad \mathbf{Y}^{(1)}_{nm}\, \mathbf{Y}^{(0)*}_{n'm'} = \mathbf{Y}^{(0)}_{nm}\, \mathbf{Y}^{(1)*}_{n'm'}\,. \qquad (38)$$

To calculate I_1 and I_2 it is necessary to carry out another expansion

$$\Phi(\theta,\varphi) = \sum_{k=0}^{\infty} \sum_{l=-k}^{k} \Phi_{kl}(\theta,\varphi)\, Y_{kl}(\theta,\varphi)\,. \qquad (39)$$

Really, in this case the integral orthogonality relations and other relationships derived in Ref. 5 yield

$$I_1 = \sum_{k=0}^{\infty} \sum_{l=-k}^{k} \Phi_{kl} \frac{(2n+1)(2n'+1)}{\sqrt{4\pi(2k+1)}} (-1)^{k+l+n'+m'+n+1} \times$$

$$\times\, C^{k0}_{n'0\,n0}\, C^{k-l}_{n'-m'\,nm} \begin{Bmatrix} k & n' & n \\ 1 & n & n' \end{Bmatrix}, \qquad (40)$$

$$I_2 = \sum_{k=0}^{\infty} \sum_{l=-k}^{k} \Phi_{kl}\, C^{k-l}_{n'-m'\,nm} (-1)^{k+l+n'+m'+n+1} \times$$

$$\times \left(\sqrt{(n'+1)(2n'+1)}\; C^{k0}_{(n'-1)0\,n0} \begin{Bmatrix} k & n'-1 & n \\ 1 & n & n' \end{Bmatrix} + \right.$$

$$\left. +\, \sqrt{n'(2n'+3)}\; C^{k0}_{(n'+1)0\,n0} \begin{Bmatrix} k & n'+1 & n \\ 1 & n & n' \end{Bmatrix} \right), \qquad (41)$$

where $C^{jm}_{j_1 m_1\, j_2 m_2}$ are the Clebsch–Gordan coefficients, and $\begin{Bmatrix} j & j_1 & j_2 \\ m & m_1 & m_2 \end{Bmatrix}$ are the Wigner $6j$–symbols.

All integrals are regular, so the optical characteristics of light scattering are calculated in terms of the amplitude functions of the scattered field.

In conclusion, we present the recursion formulas for the functions α^{q}_{n}, β^{q}_{n}, σ^{q}_{n}, η^{q}_{n}, γ^{q}_{n}, and λ^{q}_{n}:

$$\alpha^{q}_{n} = q\, j^{(q-1)}_n(\rho_{20}) + \rho_{20}\, j^{(q)}_n(\rho_{20})\,,$$

$$\sigma^{q}_{n} = \frac{1}{\rho_{20}} (j^{(q)}_n(\rho_{20}) - q\, \sigma^{q-1}_{n})\,, \qquad (42)$$

$$\beta^{q}_{n} = q\, h^{(q-1)}_n(\rho_{10}) + \rho_{10}\, h^{(q)}_n(\rho_{10})\,,$$

$$\eta^{q}_{n} = \frac{1}{\rho_{10}} (h^{(q)}_n(\rho_{10}) - q\, \eta^{q-1}_{n})\,, \qquad (43)$$

$$\gamma^{q}_{n} = q\, j^{(q-1)}_n(\rho_{10}) + \rho_{10}\, j^{(q)}_n(\rho_{10})\,,$$

$$\lambda^{q}_{n} = \frac{1}{\rho_{10}} (j^{(q)}_n(\rho_{10}) - q\, \lambda^{q-1}_{n})\,. \qquad (44)$$

One can find the recursion formulas for the Bessel and Hankel functions and for their derivatives of the qth order in Ref. 9.

3. CALCULATED RESULTS

Convergence of the PMSS method is illustrated by the data given in the tables.

Results of calculations for a spherical particle with diffraction radius $\rho = 3$ perturbed to a sphere with $\rho = 3.45$ for the refractive index $m = 1.212 + i\,0.601$ are given in Table I. The data for $\rho = 8 \to 8.4$ and $m = 1.212 + i\,0.0601$ are given in Table II.

TABLE I.

N	K_{ext}	$I(\theta = 0°)$	K_{sc}	$I(\theta = 180°)$
0	1.0841	0.865990	0.9652	0.002215
1	1.2383	1.019322	1.2345	0.001413
2	1.3129	1.091631	1.2085	0.004078
3	1.3138	1.110172	1.1696	0.002552
4	1.3101	1.113392	1.1687	0.001824
5	1.3112	1.112781	1.1779	0.001812
6	1.3124	1.112167	1.1772	0.001981
7	1.3121	1.112218	1.1732	0.001973
8	1.3119	1.112291	1.1735	0.001964
9	1.3119	1.112280	1.1749	0.001966
10	1.3120	1.112269	1.1748	0.001968
0	1.3120	1.112278	1.1745	0.001967

TABLE II.

N	K_{ext}	$I(\theta = 0°)$	K_{sc}	$I(\theta = 180°)$
0	2.7672	5.586794	1.8439	0.000386
1	2.7939	5.989660	1.9033	0.001316
2	2.7964	6.143039	1.8578	0.000887
3	2.7985	6.163910	1.8544	0.000618
4	2.7989	6.160829	1.8554	0.000652
5	2.7979	6.158985	1.8547	0.000671
6	2.7978	6.159033	1.8546	0.000669
7	2.7980	6.159237	1.8548	0.000671
8	2.7980	6.159276	1.8548	0.000671
0	2.7980	6.159270	1.8547	0.000670

The optical characteristics calculated by the Mie theory for spheres with indicated initial and final radii are given in the first and the last rows of the tables, respectively. The algorithm was tested for convergence in the example of a sphere with $r = a$ perturbed to a sphere with $r = a(1 + \varepsilon)$. The serial number of the row in the table corresponds to the order of perturbation. The values of the extinction efficiency factor are given in the second column, the values of the forward scattering phase functions are in the third column, the values of the scattering efficiency factor are in the fourth column, and the values of the backscattering phase function are in the fifth column.

As is seen from the tables, convergence of numerical estimates is reached for the given values of the initial parameters by taking into account the corrections up to eighth and tenth orders. However, even higher orders can be needed for other initial data, especially for perturbed nonspherical shape.

To illustrate the influence of the particle shape on the light scattering properties, let us present the results of the model estimations by the PMSS method for spheroid taking into account two corrections.

Representation of the three–axes ellipsoid with the half–axes $a/(1 - u\varepsilon)$, $a/(1 - v\varepsilon)$, and $a/(1 - w\varepsilon)$ as a series expansion in terms of spherical functions has the form

$$f = u\xi^2 + v\eta^2 + w\zeta^2 \,, \tag{45}$$

$$\xi = \sqrt{2\pi/3}\,\big(\exp(-i\,\psi_0)\,(\,i \sin\varphi_0 - \cos\theta_0 \cos\varphi_0)\,Y_{11} + \exp(i\,\psi_0)(i \sin\varphi_0 + \cos\theta_0 \cos\varphi_0)\,Y_{1-1} - \sqrt{2}\sin\theta_0 \cos\varphi_0\,Y_{10}\big), \tag{46}$$

$$\eta = \sqrt{2\pi/3}\,\big(\exp(-i\,\psi_0)\,(\,i \cos\varphi_0 + \cos\theta_0 \sin\varphi_0)\,Y_{11} + \exp(i\,\psi_0)(i \sin\varphi_0 + \cos\theta_0 \cos\varphi_0)\,Y_{1-1} + \sqrt{2}\sin\theta_0 \sin\varphi_0\,Y_{10}\big), \tag{47}$$

$$\xi = \sqrt{2\pi/3}\,\big(-\exp(-i\,\psi_0)\sin\theta_0\,Y_{11} + \exp(i\,\psi_0)\sin\theta_0\,Y_{1-1} + \sqrt{2}\cos\theta_0\,Y_{10}\big)\,. \tag{48}$$

The coefficients of the expansion in series in terms of spherical functions for f^k, $k = 1, 2, \ldots, p$ are found under the program based on Eqs. (46)–(48) that implements the convolution algorithm.

Angular dependence is shown in Fig. 1 for the normalized values of four elements of the scattering phase matrix at the scattering angle θ (in the plane $\varphi = 0$) that characterize the polarization properties of light scattered by a spheroid (the simplest everywhere convex shape). The analogous data for the inverted spheroid of the simplest shape with concave region (dumb–bell–shaped body) are shown in Fig. 2.

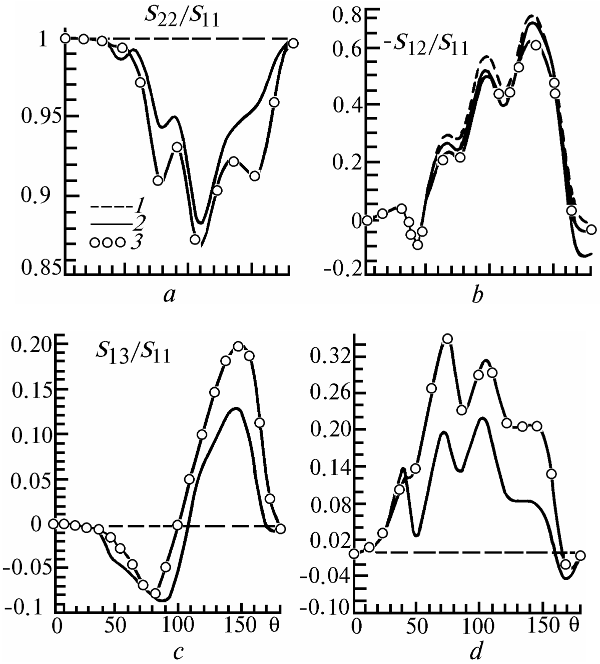

FIG. 1. Angular dependence of the normalized elements of the scattering phase matrix for a spheroid calculated by the perturbation method considering different number of corrections.

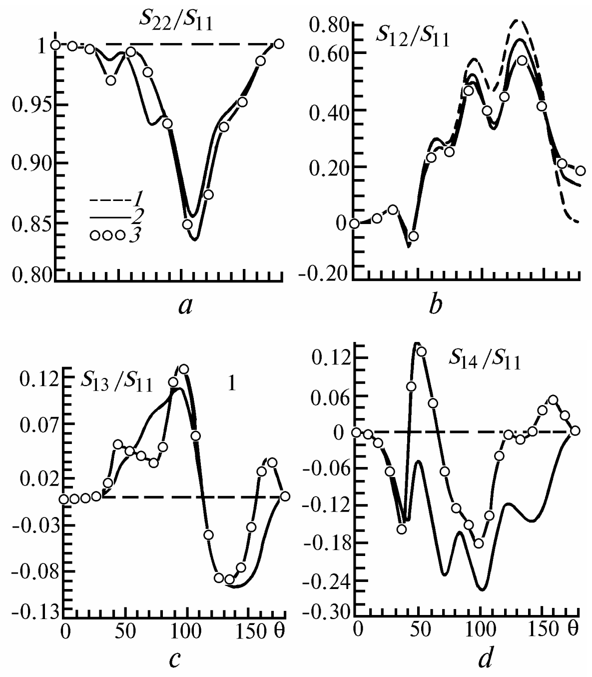

FIG. 2. The same for inverted spheroid.

The scattering particle in both cases was oriented at the Euler angles $\theta_0 = \pi/4$, $\varphi_0 = 0$, and $\psi_0 = 0$ to the incident radiation. The diffraction radius of the nonperturbed sphere was $\rho = 5$, the refractive index was $m = 1.212 + i0.0601$, $\varepsilon = 0.01$, the degree of perturbation along the half-axes was determined by the values u_ε, v_ε, and w_ε, where $u = v = 4.6544$ and $w = 10$. Incident plane light wave was linearly polarized along the x axis. Curves *1* are for the angular light scattering functions of nonperturbed sphere, curves *2* are for the calculated data taking into account only the first order of perturbation, and curves *3* are for calculations taking into account the perturbation correction of the second order.

As is seen from Figs. 1*c* and *d* and Figs. 2*c* and *d*, the elements S_{13} and S_{14} of a sphere at any θ vanish and their nonzero values characterize the degree of shape deviation from a sphere, i.e., the particle nonspherisity. Their angular behavior is essentially different for perturbation of different sign. It also should be noted that the degree of depolarization is more pronounced at small scattering angles for inverted spheroid (i.e., with concave region on its surface) than for elongated spheroid. It also should be added that the angular dependence calculated for first and second corrections has more pronounced difference for inverted spheroid than for elongated spheroid with everywhere convex surface (Figs. 2*c* and *d*).

ACKNOWLEDGMENTS

This work was supported in part by Russian Fundamental Research Foundation Grant No. 94–05–16463a.

REFERENCES

1. C. Yeh, Phys. Rev. **135**, 1193 (1964).
2. V.A. Erma, Phys. Rev. **173**, 1243 (1968).
3. V.A. Erma, Phys. Rev. **176**, 1544 (1968).
4. V.A. Erma, Phys. Rev. **179**, 1238 (1969).
5. D.A. Varshalovich, A.N. Moskalev, and V.K. Khersonskii, *Quantum Theory of Angular Momentum* (Nauka, Leningrad, 1975), 340 pp.
6. P. Barber and C. Yeh, Appl. Opt. **14**, No. 12, 2864–2872 (1975).
7. S. Asano and G. Yamamoto, Appl. Opt. **14**, No. 1, 29–49 (1975).
8. D. Jackson, *Classical Electrodynamics* [Russian translation] (Mir, Moscow, 1971), 792 pp.
9. M.I. Abramovitz and I.M. Stegun, eds., *Handbook of Mathematical Functions* (U.S.Govt. Printing Office, Washington, 1972).