METHOD OF CALCULATING THE PARAMETERS OF THE SCATTERING OF LIGHT BY A TWO–LAYER SPHERE WITH INHOMOGENEOUS SHELL

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A method is developed for calculating the parameters of the scattering of light by a two-layer sphere with homogeneous core and radially inhomogeneous shell whose complex refractive index depends on the parameter ρ *as* $m = A\rho^{b}$ *, where* $\rho = 2nr/\lambda$ *(r is the radial distance from the center of the particle,* λ *is the wavelength) and A and b are the arbitrary complex constants. The method is based on combining the Gegenbauer summation theorem and the expansion of the Bessel functions and their logarithmic derivatives in continued fraction.*

Treating theoretically the problem of the scattering of light by the dispersions, one often can be faced with a necessity of taking into account of the optical inhomogeneity of particles. In this case it became common practice to use the model of a multilayer sphere with radial nonuniformity of the refractive index. This model often appears to be inadequate to the real optical properties of the particles. This fact makes one to introduce more sophisticated models. A model of a two–layer sphere with homogeneous core and radially inhomogeneous shell was employed in the 1960's–1970's to describe the scattering properties of a number of objects being outside the field of atmospheric optics (Refs. 1 and 2).

In recent years there has been an increase in interest to this model associated with the problems of the scattering of light by partially solvable particles of an atmospheric aerosol, by evaporating particles surrounded with a vapor–gas halo, and by some artificial aerosols. The sphere with inhomogeneous shell was employed for describing the fine fraction of the ocean suspension[3,4] and for modeling the scattering of light on an ensemble of particles with random shape.[5,6] Its application to fractal clasters is the matter of particular interest.[7] Widespread adoption of this model into the calculations of the scattering of light is impeded by mathematical difficulties (not only of analytic but also of computational character).

The purpose of this paper is to construct a stable and reliable algorithm for calculating the characteristics of the scattering of light by the above-indicated variety of two–layer particles with the radial inhomogeneity of rather general form.

Let us refine the formulation of this problem. A plane monochromatic (with wavelength λ) electromagnetic wave is incident on the particle having a spherical core of a radius r with constant complex refractive index $m_1 = \hat{n} - i\kappa_1$ and concentric shell with the external radius r_2 with the refractive index $m_2(\rho) = \hat{n}_2(\rho) - i\kappa_2(\rho)$, whose the value is a function of relative distance $\rho = 2\pi r/\lambda$ to the center of the sphere. The rigorous theory of the scattering of light on such an object was developed in Ref. 8. The details of this rather complicated and cumbersone derivation need not be discussed and we shall give only the final relations for the scattering characteristics. In contrast to Ref. 8, the expressions for the amplitude coefficients of the scattered field can be written in the following form suitable for numerical calculations ($l = 1, 2, \ldots$):

$$\alpha_l = B_l \frac{E_l\gamma_{11}^{(3)}\gamma_{12}^{(1)} - \gamma_{11}^{(1)}\gamma_{12}^{(3)}}{E_l\gamma_{13}^{(3)}\gamma_{12}^{(1)} - \gamma_{13}^{(1)}\gamma_{12}^{(3)}}$$

and $$\beta_l = B_l \frac{C_l\gamma_{14}^{(3)}\gamma_{15}^{(1)} - \gamma_{14}^{(1)}\gamma_{15}^{(3)}}{C_l\gamma_{16}^{(3)}\gamma_{15}^{(1)} - \gamma_{16}^{(1)}\gamma_{15}^{(3)}}, \quad (1)$$

where $$\gamma_{11}^{(1)} = F_l^{(1)}(\rho_2) - D_l(\rho_2),$$

$$\gamma_{12}^{(1)} = F_l^{(1)}(\rho_1) - m_1 D_l(m_1\rho_2),$$

$$\gamma_{13}^{(1)} = G_l(\rho_2) - F_l^{(1)}(\rho_2),$$

$$\gamma_{14}^{(1)} = m_2^2(\rho_2)D_l(\rho_2) - R_l^{(1)}(\rho_2),$$

$$\gamma_{15}^{(1)} = \frac{m_1}{m_2^2(\rho_1)} R_l^{(1)}(\rho_1) - D_l(m_1\rho_1),$$

$$\gamma_{16}^{(1)} = R_l^{(1)}(\rho_2) - m_2^2(\rho_2)G_l(\rho_2) \quad (2)$$

(the expressions for $\gamma^{(3)}$ are derived from the corresponding expression for $\gamma^{(1)}$ by substituting $F^{(3)}$ and $R^{(3)}$ for $F^{(1)}$ and $R^{(1)}$),

$$B_l = \psi_l(\rho_2)/\xi_l(\rho_2),$$

$$C_l = W_l^{(1)}(\rho_1)W_l^{(3)}(\rho_2)/W_l^{(3)}(\rho_1)W_l^{(1)}(\rho_2),$$

and $$E_l = V_l^{(1)}(\rho_1)V_l^{(3)}(\rho_2)/V_l^{(3)}(\rho_1)V_l^{(1)}(\rho_2), \quad (3)$$

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The following notation is accepted in Eqs. (2) and (3): $\rho_{1,2} = 2\pi r_{1,2}/\lambda$ are the diffraction parameters for the core and for the shell, respectively; $\psi_l(\rho)$ and $\xi_l(\rho)$ are the Riccati–Bessel and the Riccati–Hankel functions; $D_l(\rho)$ and $G_l(\rho)$ are the logarithmic derivatives of the functions $\psi_l(\rho)$ and $\xi_l(\rho)$, respectively; $W_l(\rho)$ and $V_l(\rho)$ are the magnetic and electric radial distribution functions (the definition is given below); $R_l(\rho)$ and $F_l(\rho)$ are the logarithmic derivatives of the functions $W_l(\rho)$ and $V_l(\rho)$, respectively: the superscript (1) denotes the functions which are regular at the origin of the coordinates and tne superscript (3) denotes the functions which satisfy the condition of radiation in the far zone of diffraction. The scattering characteristics can be calculated from the standard formula[9] given that the coefficients α_l and β_l for the amplitudes are known.

Radial distribution functions $W_l^{(i)}(\rho)$ and $V_l^{(i)}(\rho)$ (i = 1, 3) are the solutions of linear differential equations of the second order

$$W_l''(\rho) - \left[\ln m_2^2(\rho)\right]' W_l'(\rho) + \left[m_2^2(\rho) - l(l+1)/\rho^2\right] W_l(\rho) = 0, \qquad (4)$$

$$V_l''(\rho) - \left[m_2^2(\rho) - l(l+1)/\rho^2\right] V_l(\rho) = 0, \qquad (5)$$

where the prime denotes the derivative with respect to ρ. A concrete form of these equations and, hence, their solution are functions of the selected profile of the refractive index $m_2(\rho)$ of the shell. As shown in Ref. 2 the analytical solutions of the radial distribution equations (4)–(5) are possible only for a very limited set of profiles $m_2(\rho)$. In this case, as a rule, the solutions are obtained in terms of hypergeometric functions which are extremely inconvenient for the numerical calculation. The only real profile which prevents from appearance of hypergeometric functions is power–law function

$$m_2(\rho) = b_1\rho^{b_2}, \qquad (6)$$

where b_1 and b_2 are the arbitrary complex constants. The particular case of profile (6) for real b_1 and b_2 was studied in Refs. 8 and 10 while a simpler case for $b_2 = -1$ was considered in Refs. 3–5 and 11. Four free parameters enter in profile (6), which makes it possible to specify independently the complex refractive indices for the interface between a core and a shell $m_2(\rho_1)$ and for the external interface of the particle $m_2(\rho_2)$. In this case the profile $m_2(\rho)$ for a shell turns out to be fixed.

Substituting Eq. (6) into radial distribution equations (4) and (5) we derive the differential equations, whose solutions are cylindrical functions

$$V_l^{(1)}(\rho) = \sqrt{\rho}\, J_{\mu_l}\left(x(\rho)\right),$$

$$V_l^{(3)}(\rho) = \sqrt{\rho}\, H_{\mu_l}^{(2)}\left(x(\rho)\right), \qquad (7)$$

$$W_l^{(1)}(\rho) = \rho^{b_2+0.5} J_{\nu_l}\left(x(\rho)\right),$$

and

$$W_l^{(3)}(\rho) = \rho^{b_2+0.5} H_{\nu_l}^{(2)}\left(x(\rho)\right), \qquad (8)$$

where J is the Bessel function and $H^{(2)}$ is the Hankel function of the second kind (below the superscript (2) is omitted). The argument x and the subscripts of these functions are equal to

$$x(\rho) = \frac{m_2(\rho)}{b_2+1}\rho,\ \mu_l = \frac{2l+1}{2(b_2+1)},\ and\ \nu_l = \frac{\sqrt{l(l+1)+(b_2+0.5)^2}}{b_2+1} \qquad (9)$$

It is obvious that functions V_l and W_l to within an unimportant constant factor transform into the Riccati–Bessel and the Riccati–Hankel functions given that a shell is homogeneous (b_2 =0). If a shell is inhomogeneous, the subscripts μ_l and ν_l are complex in the general case. As Eqs. (1)–(3) show, cylindrical functions (7) and (8) enter into the amplitude coefficients in the form of the following ratios:

$$R_l^{(1)}(\rho) = \frac{2b_2 + 1}{2\rho} + m_2(\rho) J'_{\nu_l}\left(x(\rho)\right)/J_{\nu_l}\left(x(\rho)\right), \qquad (10)$$

and

$$F_l^{(1)}(\rho) = \frac{1}{2\rho} + m_2(\rho) J'_{\mu_l}\left(x(\rho)\right)/J_{\mu_l}\left(x(\rho)\right), \qquad (11)$$

where the prime refers to the derivative with respect to the argument $x(\rho)$, $R_l^{(3)}$ and $F_l^{(3)}$ are derived from Eqs. (10) and (11) by substituting the Hankel function for the Bessel function,

$$C_l = J_{\nu_l}\left(x(\rho_1)\right) H_{\nu_l}\left(x(\rho_2)\right)/H_{\nu_l}\left(x(\rho_1)\right) J_{\nu_l}\left(x(\rho_2)\right) \qquad (12)$$

(the expression for E_l is analogous to Eq. (12) in which μ_l is substituted for ν_l). In the particular case in which b_2 = – 1 (Refs. 3, 5, and 11) radial distribution functions degenerate into the power – law functions and

$$R_l^{(1)} = -F_l^{(3)} = (q_l - 1)/2\rho,$$

$$F_l^{(1)} = -R_l^{(3)} = (q_l + 1)/2\rho,$$

$$C_l = E_l = (\rho_1\rho_2)^{q_l},\quad q_l = 2\left[(l + 0.5)^2 - b_1^2\right]^{1/2}.$$

Thus, to calculate the amplitude coefficients, it is necessary to obtain three groups of functions: 1) functions $\psi_l(\rho_2)$, $\xi_l(\rho_2)$ and logarithmic derivatives $D_l(\rho_2)$, $G_l(\rho_2)$, and $D_l(m_l, \rho_l)$; 2) logarithmic derivatives $I'_{\nu_l}(z)/I_{\nu_l}(z)$, $H'_{\nu_l}(z)/H_{\nu_l}(z)$ and ratios $I_{\nu_l}(z)/H_{\nu_l}(z)$ for the arguments $z = x(\rho_l)$ and $z = x(\rho_2)$; 3) analogous functions for different subscripts μ_l. Numerical calculation of the functions of the first group is not difficult. To estimate the number of terms L sufficient for the convergence of the series in the amplitude coefficients, we can use the relation[12]

$$L = \begin{cases} 1.01(\rho_2 + 4.05(\rho_2)^{1/3} + 2), & \rho_2 \geq 0.02 \\ 2, & \rho_2 < 0.02, \end{cases} \qquad (13)$$

primarily derived for the homogeneous spheres. The set of the logarithmic derivatives $D_l(\rho_2)$ and $D_l(m_l, \rho_l)$ (l = L, L – 1, ..., 1) is evaluated by following a procedure of backward recurrence, starting terms of recursion have been derived from the expansion in a continued fraction.[13] Functions $\xi_l(\rho_2)$ and $G_l(\rho_2)$ were calculated by forward recursion (l = 1, 2, ..., L) and functions $\psi_l(\rho_2)$ were estimated by following a procedure of backward recurrence with recalculation. A more detailed description of the technique for calculating these functions is given elsewhere.[12-14]

As to the functions of the second and third groups, the estimation of them is more complicated. One can see from Eq. (9) that it is impossible here to construct the recurrence procedure for l. This fact forces us to perform an independent calculation for every l = 1, 2, ... L. The situation is not simplified even taking into account that we need the ratios of the functions, rather than the functions themselves. In the case of complex subscripts it is impossible to obtain these ratios without performing a direct computer calculation of at least one cylindrical function. For this purpose the regular function $I_\nu(z)$ is required (to simplify notation, we subsequently consider the arbitrary argument z and the subscript ν). To calculate this function, we somewhat modified the technique proposed in Ref. 15, which is the generalization of the method described in Ref. 16, to the complex values of ν. We shall introduce the sequence of auxiliary functions $F_n(z)$ (n = 0, 1, ..., N_1^*; the definition of N_1^* is given below) which are related to the functions $I_{\nu+n}(z)$ by the normalization constant A : $AI_{\nu+n}(z) = F_n(z)$ and it then follows that these functions follow the same recursion for n as the Bessel function does:

$$F_{n-1}(z) = \frac{2(\nu+n)}{z} F_n(z) - F_{n+1}(z). \tag{14}$$

As is well known the recursion (14) is stable only in calculating the backward recursion. In this case we should start the recursion from the subscript N_1^* which is noticeably greater than not only $|\nu|$ but also $|z|$. We used the following estimate for N_1^* :

$$N_1^* = \max \begin{cases} 1.5|z| - |\nu| + 15, \\ 30, \end{cases} \tag{15}$$

rounded off to the nearest odd number. The initial values are $F_{N_{1-1}}^* = 0$ and $F_{N_1}^* = 10^{-35}(I + i)$. If the condition (15) is satisfied, the sequence $F_n(z)$ converges within 5 to 6 steps of recursion. For this reason the values of F_n with n = 0, 1, ... , $2N_1$, where $2N_1 = N_1^* - 5$, are assumed to be correct. The Gegenbauer summation theorem[17]

$$\sum_{n=0}^{\infty} \frac{(\nu + 2n)\Gamma(\nu + n)}{n!} J_{\nu+2n}(z) = \left[\frac{z}{2}\right]^\nu, \tag{16}$$

where Γ is the gamma–function, leads to the relation for the normalization constant A (the details are given in Ref. 16)

$$A = \sum_{k=0}^{\infty} \alpha_k F_{2k}(z), \tag{17}$$

where the coefficients α_k are calculated by multiplicative recursion $\alpha_k = c_k\alpha_{k-1}$, in addition $\alpha_0 = (2/z)^\nu\,\Gamma(1 + \nu)$ and $c_k = (\nu + 2k)(\nu + k - 1)/(\nu + 2k - 2)$. The summation in Eq. (17) is performed either up to $k = N_1$ or is stopped if the ratio of the subsequent term to the sum of the preceding terms in a series is smaller than 10^{-8}. The goal function $I_\nu(z)$ is equal to

$$J_\nu(z) = A^{-1}F_0(z). \tag{18}$$

In realizing this method, some difficulties have arisen. The series (17) converges rather slowly, especially for large negative value of Re ν, so that for Re $\nu < 0$ the value of $I_{-\nu}(z)$ is calculated instead of $I_\nu(z)$.

The numerical calculation of the gamma–function of the complex argument $\Gamma(1+\nu)$ gives rise to some difficulties. Standard subroutines are employed with single precision that results in either overflow or zero of the result and finally in a wrong value of α_0. Therefore, it turned out natural to rewrite the equation in logarithmic form

$$\ln\alpha_0 = \nu\ln(2/z) + \ln\Gamma(1 + \nu)$$

with subsequent reconstruction of α_0. The logarithm of the gamma–function can be calculated using a standard subroutine.

The nigh orders of magnitude appearing in calculating F_n and c_k by recursions can be avoided to a strong degree by scaling F_n to Re F_0, and α_k to α_0. After normalization, basic relation (18) can be written in the form

$$J_\nu(z) = \tilde{F}_0(z)/\alpha_0\sum_{k=0}^{N_1} \tilde{\alpha}_k \tilde{F}_{2k}(z). \tag{19}$$

The most significant difficulties are connected with the opposite directions of recursions for F and α if the domain of convergence of series (17) is *a priori* unknown. If N_1 terms of a series do not provide for the convergence by the selected criterion, we must perform an additional calculation of $\overline{F}_n$ (n = $2N_1$, $2N_1 + 1$, ..., N_2^*) using the backward recursion algorithm (14) with initial values $\overline{F}^*_{N_2+1} = 0$ and $\overline{F}^*_{N_2} = 10^{-15}(1 + i)$, where $N_2^* = 2N_1 + 15$. The sequence $\overline{F}_n$ and the previously obtained sequence $\tilde{F}_n$ can be joined together at $n = 2N_1$. If we denote the ratio $\tilde{F}_{2N_1}/\overline{F}_{2N_1}$ by f, it becomes obvious that the sequence $\tilde{F}_{2N_1+1} = f\overline{F}_{2N_1+1}$, ..., $\tilde{F}_{2N_2} = f\overline{F}_{2N_2}$ (where $2N_2 = N_2^* - 5$) is scaled analogous to the primary one. Hence, after the values c_k ($\kappa = N_1 + 1$, ..., N_2) have been obtained by recursion we can continue the summation in the denominator of Eq. (19). If the convergence is not provided, the procedure must be repeated.

Based on the Gegenbauer summation theorem, the method for calculating $I_\nu(z)$ permits one to estimate simultaneously the value of the logarithmic derivative

$$D_\nu(z) \equiv \frac{J'_\nu(z)}{J_\nu(z)} = -\frac{\tilde{F}_1(z)}{\tilde{F}_0(z)} + \frac{\nu}{z}. \tag{20}$$

Moreover, this method makes it possible to calculate the Neuman function $Y_\nu(z)$. It was shown in Ref. 16 that

$$Y_\nu(z) = A^{-1}\sum_{k=0}^{\infty} \beta_k F_{2k}(z), \tag{21}$$

where

$$\beta_k = c_k \beta_{k-1}(2\nu + k - 1)/(\nu - k), \quad k = 2, 3, \ldots$$

$$\beta_0 = \cot\nu\pi - \alpha_0^2/\nu\pi, \quad \beta_1 = 2\alpha_0^2(\nu + 2)/\pi(\nu - 1).$$

To obtain the desirable relations (using the Wronskian and the relations for the derivatives), it is quite sufficient to know I_ν, Y_ν and D_ν. However, the calculations indicated that this way of calculating Y_ν is numerically stable only for $|\nu| \gg |z|$. If $|\nu| \ll |z|$ (as a rule, this occurs when the series (21) is summarized), a dramatic loss of precision occurs. Given that the subscript and the argument are of the same order of magnitude, the loss of precision is small, but an extremely slow convergence of series (21) is observed. Therefore, we employed another approach. As is well known, the expansion of the relation $I'_\nu(z)/I_\nu(z)$ in a continuous fraction for a half–integer ν is widely used in modern algorithms for calculations using the Mie theory.[12,13] This expansion is quite stable in the numerical aspect; a slight modification enables us to employ it to the complex subscripts and to the calculation of $D_{-\nu}(z)$(Re ν > 0). For Re ν < 0, this method is employed for the calculation of $D_\nu(z)$.

Further, we obtain from the well–known Wronskian

$$M_\nu(z) \equiv \frac{J_{-\nu}(z)}{J_\nu(z)} = \left[\frac{2\sin\nu\pi}{\pi z} \times \frac{1}{J^2_{\pm\nu}(z)\left[D_\nu(z) - D_{-\nu}(z)\right]}\right]^{\pm 1} \quad (22)$$

(upper signs refer to Re ν > 0, lower signs refer to Re ν < 0). The expressions for the ratios sought follow from the definition of the Hankel functions

$$\frac{H'_\nu(z)}{H_\nu(z)} = D_\nu(z) + \frac{M_\nu(z)}{K_\nu(z)}\left[D_\nu(z) - D_{-\nu}(z)\right]$$

and $\dfrac{J_\nu(z)}{H_\nu(z)} = \dfrac{i\sin\nu\pi}{K_\nu(z)}$,

where

$$K_\nu(z) = e^{i\nu\pi} - M_\nu(z).$$

The developed algorithm was implemented on a BESM–6 computer. The test calculations show an agreement with the results given in Refs. 10 and 11 for degenerated cases. A version of this program for polydispersions (lognormal and gamma distributions of radius r of the core and the constant ratio of external radius r_2 to r_1) was employed for studying characteristics of the scattering of light on clasters and different types of the atmospheric aerosol.

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