

TECHNIQUE FOR CALCULATING THE INTERNAL FIELD OF A TWO-LAYER SPHERICAL PARTICLE WITH INHOMOGENEOUS SHELL

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A stable and reliable algorithm is constructed for computing the internal field of a two-layer spherical particle with homogeneous core and radially inhomogeneous shell whose inhomogeneity profile is described by a power-law function. This model is intended for calculating the interaction of the electromagnetic wave with fractal clusters in the framework of the asymptotic cluster model.

In recent years the great interest has been expressed in optics of fractal clusters, specifically in calculation of optical characteristics of soot agglomerates formed in the atmosphere by a stochastic association of primordial subparticles — combustion products — into larger friable formations of micron size (see, for example, Refs. 1–4). Construction of an adequate model of the object describing optical properties of fractals is a problem of principle. A so-called asymptotic model of a cluster in the form of a two-layer sphere with homogeneous core and radially inhomogeneous shell was proposed in Ref. 5. Such a model makes it possible to describe more or less adequately the actual dependence of the refractive index of the shell on the radial coordinate; on the other hand, the diffraction problem has an exact solution in terms of special functions given that the profile of the refractive index is chosen properly. A technique for calculating the characteristics of light scattering by such objects was described in Ref. 6 and the calculated results were presented in Refs. 7 and 8.

However, knowledge of the field distribution inside the cluster is required for a closer study of an interaction between electromagnetic wave and fractal clusters. In particular, the local field parameters calculated within the scope of this model can facilitate a solution of the problem on the supposed sharp decrease of nonlinearity threshold.⁹ They also determine the regions of the most active interaction.

The model of the radially inhomogeneous sphere has drawn interest in the calculation of heating of soot structures formed as a result of combustion of coal particles in gaseous phase^{10,11} and of haloes surrounding the evaporating particles. Moreover, knowledge of the internal field provides a description of scattering patterns of inhomogeneous and anisotropic particles as well as of particles with nonlinear properties in the framework of the integral equation method¹² in which the potential of the radially inhomogeneous particle is used as a seed potential of interaction.

Mathematical difficulties (both analytical and computational) are a barrier to a widespread use of the model; that is why the papers devoted to the internal field of the radially inhomogeneous particles are practically lacking (except Ref. 13). The goal of the present paper is construction of a stable and reliable algorithm for calculating the internal field of the above-indicated variety of two-layer particles with radially inhomogeneous profile of the refractive index of a sufficiently general type.

Let us particularize the statement of the problem. A plane monochromatic ($e^{i\omega t}$) electromagnetic wave (with wavelength λ and amplitude E_0 propagating in the positive

direction along the z axis, whose electric vector oscillates about the x axis) is incident on a particle having a spherical core of relative radius $\rho_1 = 2\pi r_1/\lambda$ (r_1 is the radius of the core) with the constant complex refractive index m_1 and a concentric shell of relative radius $\rho_2 = 2\pi r_2/\lambda$ (r_2 is the external radius of the particle), whose refractive index $m_2(\rho)$ depends on the relative distance ρ from the center of the sphere. Vector wave functions $\mathbf{M}_{onl}^{(j)}(m\rho)$ and $\mathbf{N}_{onl}^{(j)}(m\rho)$

($l = 1, 2, \dots, n = 0, 1, \dots, l$) are known to be the solutions of the vector wave equations¹¹ for homogeneous region. Here the functions with the superscript $j = 1$ are regular at the origin of coordinate, and the functions with $j = 3$ satisfy the condition of radiation in the far zone of diffraction. The subscripts e and o denote even and odd functions, respectively. The expansions of electric and magnetic fields inside the homogeneous core ($\mathbf{E}_1, \mathbf{H}_1$) and outside of the core ($\mathbf{E}_3, \mathbf{H}_3$) for the chosen geometry of the problem have the form¹⁴

$$\begin{aligned} \mathbf{E}_1 &= \sum_{l=1}^{\infty} \varepsilon_l \left[\alpha_{1l} \mathbf{M}_{o1l}^{(1)}(m_1 \rho) + i \beta_{1l} \mathbf{N}_{e1l}^{(1)}(m_1 \rho) \right], \\ \mathbf{H}_1 &= \sqrt{\frac{\varepsilon_0}{\mu_0}} m_1 \sum_{l=1}^{\infty} \varepsilon_l \left[-\beta_{1l} \mathbf{M}_{e1l}^{(1)}(m_1 \rho) + i \alpha_{1l} \mathbf{N}_{o1l}^{(1)}(m_1 \rho) \right], \\ \mathbf{E}_3 &= \sum_{l=1}^{\infty} \varepsilon_l \left[\mathbf{M}_{o1l}^{(1)}(\rho) + \alpha_{4l} \mathbf{M}_{o1l}^{(3)}(\rho) + \right. \\ &\quad \left. + i \mathbf{N}_{e1l}^{(1)}(\rho) + i \beta_{4l} \mathbf{N}_{e1l}^{(3)}(\rho) \right], \\ \mathbf{H}_3 &= \sqrt{\frac{\varepsilon_0}{\mu_0}} \sum_{l=1}^{\infty} \varepsilon_l \left[-\mathbf{M}_{e1l}^{(1)}(\rho) - \beta_{4l} \mathbf{M}_{e1l}^{(3)}(\rho) + \right. \\ &\quad \left. + i \mathbf{N}_{o1l}^{(1)}(\rho) + i \alpha_{4l} \mathbf{N}_{o1l}^{(3)}(\rho) \right], \end{aligned} \quad (1)$$

where $\varepsilon_l = (-i)^l (2l + 1) / l(l + 1)$; ε_0 and μ_0 are the dielectric constant and the magnetic permeability; unimportant factor $E_0 e^{i\omega t}$ is omitted from here on; and, α_{1l} , β_{1l} , α_{4l} , and β_{4l} are the amplitude coefficients.

More complicated is the problem for inhomogeneous region of the shell ($\rho_1 < \rho < \rho_2$). As shown in Ref. 12, elementary vector solutions to the wave equation

$$\nabla \times \nabla \times \mathbf{E}_2 - \kappa_0^2 m_2^2(\rho) \mathbf{E}_2 = 0 \tag{2}$$

are the vector functions

$$\begin{aligned} {}^{(e)}\mathbf{M}_{e_{nl}}^{(j)} &= \frac{1}{\rho} V_l^{(j)}(\rho) \mathbf{m}_{e_{nl}}, \\ {}^{(e)}\mathbf{N}_{e_{nl}}^{(j)} &= \frac{1}{m_2^2(\rho) \rho} \left[\frac{1}{\rho} W_l^{(j)}(\rho) \mathbf{l}_{e_{nl}} + W_l^{(j)'}(\rho) \mathbf{n}_{e_{nl}} \right], \end{aligned} \tag{3}$$

and to the wave equation

$$\nabla \times \nabla \times \mathbf{H}_2 - \frac{\nabla m_2(\rho)}{m_2^2(\rho)} [\nabla \times \mathbf{H}_2] - \kappa_0^2 m_2^2(\rho) \mathbf{H}_2 = 0 \tag{4}$$

are the wave functions

$$\begin{aligned} {}^{(h)}\mathbf{M}_{e_{nl}}^{(j)} &= \frac{1}{\rho} W_l^{(j)}(\rho) \mathbf{m}_{e_{nl}}, \\ {}^{(h)}\mathbf{N}_{e_{nl}}^{(j)} &= \frac{1}{\rho} \left[\frac{1}{\rho} V_l^{(j)}(\rho) \mathbf{l}_{e_{nl}} + V_l^{(j)'}(\rho) \mathbf{n}_{e_{nl}} \right]. \end{aligned} \tag{5}$$

The following notation is used here: \mathbf{l} , \mathbf{m} , and \mathbf{n} are the angular vector wave functions,¹² primes denote differentiation with respect to ρ , the meaning of the superscript j remains the same as earlier, and the radial functions W_l and V_l are the solutions of the linear differential equations of the second order

$$W_l''(\rho) - \frac{d}{d\rho} [\ln m_2^2(\rho)] W_l'(\rho) + \left[m_2^2(\rho) - \frac{l(l+1)}{\rho^2} \right] W_l(\rho) = 0, \tag{6}$$

$$V_l''(\rho) + \left[m_2^2(\rho) - \frac{l(l+1)}{\rho^2} \right] V_l(\rho) = 0. \tag{7}$$

Expansion of the field inside the shell (\mathbf{E}_2 , \mathbf{H}_2) must include not only regular ($j = 1$) but also irregular ($j = 3$) functions.

In accordance with this

$$\begin{aligned} \mathbf{E}_2 &= \sum_{l=1}^{\infty} \varepsilon_l \left[\alpha_{2l}^{(e)} \mathbf{M}_{o1l}^{(1)}(\rho) + \alpha_{3l}^{(e)} \mathbf{M}_{o1l}^{(3)}(\rho) + \right. \\ &+ \left. i \beta_{2l}^{(e)} \mathbf{N}_{e1l}^{(1)}(\rho) + i \beta_{3l} \mathbf{N}_{e1l}^{(3)}(\rho) \right], \\ \mathbf{H}_2 &= \sqrt{\frac{\varepsilon_0}{\mu_0}} \sum_{l=1}^{\infty} \varepsilon_l \left[-\beta_{2l}^{(h)} \mathbf{M}_{e1l}^{(1)}(\rho) - \beta_{3l}^{(h)} \mathbf{M}_{e1l}^{(3)}(\rho) + \right. \\ &+ \left. i \alpha_{2l}^{(h)} \mathbf{N}_{o1l}^{(1)}(\rho) + i \alpha_{3l}^{(h)} \mathbf{N}_{o1l}^{(3)}(\rho) \right], \end{aligned} \tag{8}$$

where α_{2l} , α_{3l} , β_{2l} , and β_{3l} are the amplitude coefficients of the field inside the shell. In order to determine the amplitude coefficients entering into Eqs. (1) and (8), the boundary conditions that the tangential components of fields are continuous at two interfaces should be used. As a result, we obtain two systems of linear algebraic equations for the amplitude coefficients. Solving these systems for the amplitude coefficients of the shell (later on we restrict ourselves to this case alone), as a result of quite

cumbersome transformations we obtain the following expressions:

$$\alpha_{2l} = i \tau_{4l} / \zeta_l(\rho_2) V_l^{(1)}(\rho_2) M_l, \tag{9}$$

$$\beta_{2l} = -i (m_2^2(\rho_2) \bar{\tau}_{4l} / \zeta_l(\rho_2) W_l^{(1)}(\rho_2) \bar{M}_l,$$

$$\alpha_{3l} = -\frac{V_l^{(1)}(\rho_1)}{V_l^{(3)}(\rho_1)} \frac{i \tau_{3l}}{\zeta_l(\rho_2) V_l^{(1)}(\rho_2) M_l}, \tag{10}$$

$$\beta_{3l} = -\frac{W_l^{(1)}(\rho_1)}{W_l^{(3)}(\rho_1)} \frac{i m_2^2(\rho_2) \bar{\tau}_{3l}}{\zeta_l(\rho_2) W_l^{(1)}(\rho_2) \bar{M}_l},$$

where

$$M_l = \tau_{1l} \tau_{4l} - E_l \tau_{2l} \tau_{3l}, \bar{M}_l = -\bar{\tau}_{1l} \bar{\tau}_{4l} - c_l \bar{\tau}_{2l} \bar{\tau}_{3l}, \tag{11}$$

$$\begin{pmatrix} \tau_{1l} \\ \tau_{2l} \end{pmatrix} = \begin{pmatrix} F_l^{(1)}(\rho_2) \\ F_l^{(3)}(\rho_2) \end{pmatrix} - G_l(\rho_2),$$

$$\begin{pmatrix} \bar{\tau}_{1l} \\ \bar{\tau}_{2l} \end{pmatrix} = \begin{pmatrix} R_l^{(1)}(\rho_2) \\ R_l^{(3)}(\rho_2) \end{pmatrix} - m_2^2(\rho_2) G_l(\rho_2),$$

$$\begin{pmatrix} \tau_{3l} \\ \tau_{4l} \end{pmatrix} = \begin{pmatrix} F_l^{(1)}(\rho_1) \\ F_l^{(3)}(\rho_1) \end{pmatrix} - m_1 D_l(m_1 \rho_2),$$

$$\begin{pmatrix} \bar{\tau}_{3l} \\ \bar{\tau}_{4l} \end{pmatrix} = \frac{m_1}{m_2^2(\rho_1)} \begin{pmatrix} R_l^{(1)}(\rho_1) \\ R_l^{(3)}(\rho_1) \end{pmatrix} - D_l(m_1 \rho_2), \tag{12}$$

$D_l(z)$ and $G_l(z)$ are the logarithmic derivatives of the Riccati-Bessel $\psi_l(z)$ and Riccati-Hankel $\zeta_l(z)$ functions, respectively,

$$R_l^{(1,3)}(\rho) = W_l^{(1,3)'}(\rho) / W_l^{(1,3)}(\rho),$$

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

$$F_l^{(1,3)}(\rho) = V_l^{(1,3)'}(\rho) / V_l^{(1,3)}(\rho),$$

$$E_l = V_l^{(1)}(\rho_1) V_l^{(3)}(\rho_2) / V_l^{(3)}(\rho_1) V_l^{(1)}(\rho_2). \tag{13}$$

In the derivation of expressions (9)–(13), the Wronskians¹⁵

$$W_l^{(1)}(r) W_l^{(3)'}(\rho) - W_l^{(1)'}(\rho) W_l^{(3)}(\rho) = i m_2^2(\rho),$$

$$V_l^{(1)}(\rho) V_l^{(3)'}(\rho) - V_l^{(1)'}(\rho) V_l^{(3)}(\rho) = i$$

were used. Let us turn back to expansions (8) for the field inside the inhomogeneous shell. Using the following designations:

$$d_{1l} = \beta_{1l} W_l^{(1)}(\rho) + \beta_{3l} W_l^{(3)}(\rho), d_{2l} = \alpha_{2l} V_l^{(1)}(\rho) + \alpha_{3l} V_l^{(3)}(\rho),$$

$$d_{3l} = \beta_{2l} W_l^{(1)'}(\rho) + \beta_{3l} W_l^{(3)'}(\rho), \tag{14}$$

we may write the components of the field \mathbf{E}_2 in spherical coordinates (r, θ, φ) in the form

$$E_{2r} = -\frac{\cos \varphi \sin \theta}{m_2^2(\rho) \rho^2} \sum_{l=1}^{\infty} (-i)^{l+1} (2l+1) Q_l(\theta) d_{1l},$$

$$\begin{pmatrix} E_{2\theta} \\ -E_{2\varphi} \end{pmatrix} = \frac{\cos \varphi}{\rho} \sum_{l=1}^{\infty} \varepsilon_l \left[\begin{pmatrix} Q_l(\theta) \\ S_l(\theta) \end{pmatrix} d_{2l} + \frac{i}{m_2^2(\rho)} \begin{pmatrix} S_l(\theta) \\ Q_l(\theta) \end{pmatrix} d_{3l} \right], \quad (15)$$

where $Q_l(\theta)$ and $S_l(\theta)$ are the angular functions expressed in terms of the associated Legendre polynomials $Q_l(\theta) = P_l^{(1)}(\cos \theta) / \sin \theta$ and $S_l(\theta) = dP_l^{(1)}(\cos \theta) / d\theta$.

Dimensionless ratio $|E|^2$ at a fixed point of the particle to the incident wave power E_0^2 is an actually computable quantity. Since the factor E_0 was omitted earlier, the ratio might be assumed equal to

$$B = E_{2r} E_{2r}^* + E_{2\theta} E_{2\theta}^* + E_{2\varphi} E_{2\varphi}^*. \quad (16)$$

At this point the construction of the formal procedure for the solution of the problem on the external field of a two-layer particle with homogeneous core and radially inhomogeneous shell is completed. However, the question of radial functions W_l and V_l remains to be solved. The concrete form of radial equations (6)–(7) and, consequently, of their solutions W_l and V_l depends on a choice of the refractive index profile $m_2(\rho)$ in the shell. As shown in Ref. 12, the radial equations are solvable analytically only for a very limited set of profiles $m_2(\rho)$. In this case the solutions are expressed, as a rule, in terms of hypergeometrical functions, which are inconvenient for computations. The only actual profile of $m_2(\rho)$, which allows one to avoid the hypergeometrical functions, is the power-law function

$$m_2(\rho) = A \rho^b, \quad (17)$$

where A and b are the arbitrary complex constants. The additional merit of the profile given by Eq. (17) is that it enables one to describe adequately the peculiarities of the optical constants at the periphery of a cluster.^{7,8} After substituting profile (17) into radial equations (6)–(7), we obtain differential equations with the following cylindrical functions as solutions:

$$\begin{pmatrix} V_l^{(1)}(\rho) \\ V_l^{(3)}(\rho) \end{pmatrix} = \sqrt{\rho} \begin{pmatrix} J_{\mu_l}(X) \\ H_{\mu_l}^{(3)}(X) \end{pmatrix}, \quad (18)$$

$$\begin{pmatrix} W_l^{(1)}(\rho) \\ W_l^{(3)}(\rho) \end{pmatrix} = \rho^{b+1/2} \begin{pmatrix} J_{\nu_l}(X) \\ H_{\nu_l}^{(2)}(X) \end{pmatrix},$$

where J is the Bessel function, $H^{(2)}$ is the Hankel function of the second kind (superscript (2) is omitted from here on). The argument X and subscripts of these functions are

$$X(\rho) = \frac{\rho m_2(\rho)}{b+1}, \quad \mu_l = \frac{2l+1}{2(b+1)}, \quad \nu_l = \frac{[l(l+1) + (b+1/2)^2]^{1/2}}{b+1}. \quad (19)$$

It is evident that for homogeneous shell ($b = 0$) the functions V_l and W_l are transformed into the Riccati–Bessel and

Riccati–Hankel functions to within the unimportant constant factor. For the inhomogeneous shell the subscripts μ_l and ν_l are complex in the general case. By substituting solution (18) into expressions (14) for the coefficients after simple transformations we obtain

$$d_{1l} = -\bar{\lambda}_l [\bar{\tau}_{4l} - \bar{\tau}_{3l} K_{\nu_l}(X_1) / K_{\nu_l}(X)],$$

$$d_{2l} = \lambda_l [\tau_{4l} - \tau_{3l} K_{\mu_l}(X_1) / K_{\mu_l}(X)],$$

$$d_{3l} = \frac{2b+1}{2r} d_{1l} - \bar{\lambda}_l m_2(\rho) \left[\bar{\tau}_{4l} D_{\nu_l}(X) - \bar{\tau}_{3l} \frac{K_{\nu_l}(X_1)}{K_{\nu_l}(X)} G_{\nu_l}(X) \right], \quad (20)$$

where

$$\lambda_l = \frac{i}{M_l \zeta_l(r_2)} \sqrt{\frac{\rho}{\rho_2}} \frac{I_{\mu_l}(X)}{I_{\mu_l}(X_2)}; \quad K_{\nu_l, \mu_l}(z) = \frac{I_{\nu_l, \mu_l}(z)}{H_{\nu_l, \mu_l}(z)},$$

$$\bar{\lambda}_l = \frac{i m_2^2(\rho_2)}{\bar{M}_l \bar{\zeta}_l(\rho_2)} \left(\frac{\rho}{\rho_2} \right)^{b+1/2} \frac{I_{\nu_l}(X)}{I_{\nu_l}(X_2)}, \quad X_{1,2} = \frac{m_2(\rho_{1,2})}{b+1} \rho_{1,2}, \quad (21)$$

M_l and \bar{M}_l are described by expressions (11) with $C_l = K_{\nu_l}(X_1) / K_{\nu_l}(X_2)$, $E_l = K_{\mu_l}(X_1) / K_{\mu_l}(X_2)$, auxiliary coefficients τ_l and $\bar{\tau}_l$ take the form

$$\begin{pmatrix} \tau_{1l} \\ \tau_{2l} \end{pmatrix} = \frac{1}{2\rho_2} - G_l(\rho_2) + m_2(\rho_2) \begin{pmatrix} D_{\mu_l}(X_2) \\ G_{\mu_l}(X_2) \end{pmatrix},$$

$$\begin{pmatrix} \tau_{3l} \\ \tau_{4l} \end{pmatrix} = \frac{1}{2\rho_1} - m_l D_l(m_l, \rho_1) + m_2(\rho_1) \begin{pmatrix} D_{\mu_l}(X_1) \\ G_{\mu_l}(X_1) \end{pmatrix},$$

$$\begin{pmatrix} \bar{\tau}_{1l} \\ \bar{\tau}_{2l} \end{pmatrix} = \frac{2b+1}{2\rho_2} - m_2^2(\rho_2) G_l(\rho_2) + m_2(\rho_2) \begin{pmatrix} D_{\nu_l}(X_2) \\ G_{\nu_l}(X_2) \end{pmatrix},$$

$$\begin{pmatrix} \bar{\tau}_{3l} \\ \bar{\tau}_{4l} \end{pmatrix} = \frac{m_1}{m_2^2(\rho_1)} \left[\frac{2b+1}{2\rho_1} + m_2(\rho_1) \begin{pmatrix} D_{\nu_l}(X_1) \\ G_{\nu_l}(X_1) \end{pmatrix} \right] - D_l(m_l, \rho_1);$$

and D_{ν_l, μ_l} and G_{ν_l, μ_l} are the logarithmic derivatives of the functions J_{ν_l, μ_l} and H_{ν_l, μ_l} , respectively.

Thus, in order to calculate the internal field of the shell, four groups of functions should be determined: (1) functions $\zeta_l(\rho_2)$ and logarithmic derivatives $G_l(\rho_2)$ and $D_l(m_l, \rho_2)$, (2) angular functions Q_l and S_l , (3) functions J_{ν_l} , logarithmic derivatives D_{ν_l} , and G_{ν_l} , and ratios K_{ν_l} for fixed arguments X_1 and X_2 and running X , and (4) analogous functions for a set of the subscripts μ_l . The calculation of functions of the first two groups is not difficult. In order to assess the number of terms L sufficient for convergence of series (15), the relation $L = fL_W$ can be used, where L_W is the assessment of the number of terms of the Mie series according to Ref. 16 and f is the empirical coefficient exceeding unity. The appearance of f is due to

the fact that the convergence of the series in the amplitude coefficients of the internal field is somewhat slower than that in the external field coefficients, for which the assessment L_W was first introduced. Our experience in the calculation of the internal field shows that $f \sim 1.2$. A set of the logarithmic derivatives $D_l(m_l \rho_l)$ ($l = L, L-1, \dots, 1$) was calculated by a backward recursion. The starting terms of recursions were obtained by the expansion in a continued fraction.¹⁷ The functions $\zeta_l(\rho_2)$ and $C_l(\rho_2)$ were calculated by a conventional forward recursion.¹⁴ The angular functions $Q_l(\theta)$ and $S_l(\theta)$ were calculated in a similar way.

Much more difficult problem is the calculation of the functions of the third and fourth groups. As can be seen from Eq. (19), construction of the recursion in l is impossible in this case; therefore, the independent calculation for every $l = 1, 2, \dots, L$ should be made. In order to calculate simultaneously the Bessel function $J_\nu(z)$ with complex subscript ν , logarithmic derivatives D_ν and G_ν , and ratio K_ν , we must somehow modify the method proposed in Refs. 18 and 19. Since this method was described in detail in Ref. 6, here we restrict our consideration to some comments. The basis of the method is the Gegenbauer addition theorem, which makes it possible to obtain $J_\nu(z)$ and $D_\nu(z)$ simultaneously. However, the simultaneous calculation of the Neumann function $Y_\nu(z)$ proposed in Ref. 19 turned out to be numerically unstable. For this reason we used another approach. As is well known, the expansion of the ratio $D_l(z)$ in a continued fraction is very stable numerically.¹⁷ A slight modification allows us to use this expansion for complex subscripts and to calculate $D_\nu(z)$. Furthermore, with the help of a combination of the known expressions for Wronskians we obtain $G_\nu(z)$ and $K_\nu(z)$ from $J_\nu(z)$, $D_\nu(z)$, and $D_{-\nu}(z)$. The developed algorithm was implemented on a BESM-6 computer. Test calculations showed an agreement with the results obtained for degenerated cases. The results of calculation of the internal field of fractals based on the developed algorithm will be presented in future papers.

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