COMPUTATION OF THE OPTICAL FIELDS INSIDE A PARTICLE BY THE MIE THEORY WITHOUT ANY RESTRICTION ON THE DIFFRACTION PARAMETER AND COMPLEX REFRACTIVE INDEX OF THE PARTICLE MATERIAL

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An algorithm for calculating the ratio of the Riccati–Bessel functions of the first kind for two values of the complex argument is constructed. It allows one to construct a system of equations for computing the optical field inside a spherical particle by the Mie theory. This algorithm removes all limitations on the values of the diffraction parameter and complex refractive index of the particle material.

The components of the optical fields inside a spherical particle are described by the Mie series, each term of which is a functional of the angular functions and of the spherical Riccati–Bessel functions (RBF) of the first kind of the complex argument and of the third kind of the real argument.[1,2] The summation of the infinite Mie series and the computations of the RBF of the third kind and of the angular functions are not difficult and do not limit the range of values of the parameters of the particle or the radiation in which the calculations can be performed in the Mie theory. At the same time the calculation of the RBF of the first kind of the complex argument $z = r + i\mu$ leads to an overflow of the machine number 10^{75} when the modulus of the imaginary part of the complex refractive index does not satisfy the condition[3]

$$| I_m(z) | < 30. \qquad (1)$$

The maximum values of the argument z are equal to the product of the diffraction parameter $\rho = 2\pi a\lambda^{-1}$ and the complex refractive index $m = n - i\kappa$ of the material of the particle. Therefore condition (1) for $\rho \gg 10^2$ can be satisfied only when $\kappa \ll 1$. This fact impeded the investigation of the optical fields not only inside plasma clusters and large metal blobs, but also inside water droplets if $\rho\kappa \geq 100$. To calculate the RBF of the first kind of the complex argument, the method of counter recursions is widely used, which assumes holding the array of RBF values, whose dimensions are somewhat larger than the product of the particle diffraction parameter and the modulus of the complex refractive index of the particle material, in the main memory. This imposes another restriction on the ranges of the values of ρ and m in which the calculations can be performed by the Mie theory. This restriction can be written as

$$\rho | m | < N_p, \qquad (2)$$

where N_p is the maximum dimension of the complex number array located in the main memory of the computer. This paper is aimed at eliminating restrictions (1) and (2) on the diffraction parameter and the complex refractive index of the particle material. Following the well-known formulas[1,2] for the Mie series which describe the complex components of the optical field intensity at the point (r, φ, θ) inside a homogeneous spherical particle, we obtain the following system of equations:

$$E_r = \frac{E_0 \sin\theta\cos\varphi}{k_i^2 r^2} \sum_{l=1}^{\infty} l(l+1) D_l Q_l(\theta); \qquad (3)$$

$$E_\eta = \frac{E_0 \cos\varphi}{k_i r} \sum_{l=1}^{\infty} \{ D_l S_l(\theta) A_l(k_i r) + i E_l Q_l(\theta) \}; \qquad (4)$$

$$E_\varphi = \frac{E_0 \sin\varphi}{k_i r} \sum_{l=1}^{\infty} \{ D_l Q_l(\theta) A_l(k_i r) + i E_l S_l(\theta) \}; \qquad (5)$$

where

$$D_l = i^l \frac{2l+1}{l(l+1)} \frac{m F_l(k_i r, m\rho)}{\xi_l(\rho) A_l(m\rho) - m\xi_l'(\rho)}; \qquad (6)$$

$$E_l = i^l \frac{2l+1}{l(l+1)} \frac{m F_l(k_i r, m\rho)}{m\xi_l(\rho) A_l(m\rho) - \xi_l'(\rho)}; \qquad (7)$$

$$F_{l+1}(z_1, z_2) = F_l(z_1, z_2) z_2 \beta_l(z_1) [z_1 \beta_l(z_2)]^{-1}; \qquad (8)$$

$$F_0(z_1, z_2) = \begin{cases} 0, & |\mu_1 - \mu_2| \geq 140, \\ \dfrac{\sin z_1}{\sin z_2}, & |\mu_1| < 140, \ |\mu_2| < 140, \\ [\cos(r_1 - r_2) + i\sin(r_1 - r_2)]\exp(\mu_1 - \mu_2), & \\ |\mu_1| \geq 140, |\mu_2| \geq 140, |\mu_1 - \mu_2| \geq 140, & \end{cases} \qquad (9)$$

$$\beta_l(z) = 2l + 1 - \alpha_l(z); \qquad (10)$$

$$\alpha_l(z) = z \frac{\varphi_{l-1}(z)}{\varphi_l(z)} = (2l+1) \times$$

$$\times \frac{z^2}{2l + 3 - [z^2/(2l + 5 - \ldots)]}; \qquad (11)$$

$$A_l(z) = -\frac{l}{z} + \left[\frac{l}{z} - A_{l-1}(z) \right]^{-1}, \quad l < \frac{1}{3}|z| + 1, \qquad (12)$$

$$A_l(z) = [\alpha_l(z) - l] z^{-1}, \quad l \geq \frac{1}{3}|z| + 1, \qquad (13)$$

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$$A_0(z) = \begin{cases} \cot z, & |\mu| < 140, \\ (0,\ i), & \mu < -140, \\ (0,\ -i), & \mu > 140. \end{cases} \quad (14)$$

The limitation imposed on the modulus of the imaginary part of Eqs. (9) and (14) is caused, on the one hand, by the falling of the exponential functions of the form $\exp(\pm\mu)$ outside the limits of the machine number for the quadruple precision of the complex number and, on the other, by violation of the criterion for accuracy of the calculations of the Bessel function written in the form of a series sum. The remaining notation is taken from Ref. 4. To calculate the RBF of the third kind, we employed forward recursion[4] with quadruple precision. The angular functions were computed using recursion relations.[5] The function $F_l(z_1, z_2)$ is equal to the ratio of the RBFs of the first order $\varphi_l(z_1)\ \varphi_l^{-1}(z_2)$. Expressions (8) and (9) eliminate overflow of the machine number 10^{75} for arbitrary κ. The forward recursion (12) for small l, for which there is no risk of unstable computations, and Eq. (13) for large l, which allows us to determine $A_l(z)$ from the value of the continued fraction (11), both of which are employed for computing the logarithmic derivative, eliminate the need for holding the entire array of the results of calculation of $A_l(z)$ in memory. Thus the computational algorithm (13)–(14) enables one to perform calculations for arbitrary ρ and m. In this case the computations for large ρ, e.g., for $\rho \sim 10^6$, are restricted only by limitations on computing time. Relations (11)–(14) allow us to calculate the scattering phase function, and the cross sections and efficiency factors for arbitrary ρ and m. It is possible to generalize the program to the case in which there are no restrictions on particle size.

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