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OPTICAL FIELD AT THE CENTER OF A SPHERE

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The paper gives an exact formula for determining the intensity of an optical field at the center of a spherical particle of arbitrary radius obtained by evaluating an indeterminate form of the 0/0 type of Mie theory for the electric-field components at the center of the sphere. This formula is valid for arbitrary values of the complex refractive index of the particle material and arbitrary wavelengths of the incident radiation. An approximation for large particles and two approximations for particle sizes less than 10^{-4} cm are obtained. The solution obtained for the optical-field intensity at the center of small particles coincides with the classical Lorentz formula for local fields.

Mie theory is inappropriate for calculating the optical-field intensity at the center of a spherical particle because in this case, Mie series contain an indeterminate form of the 0/0 type. Accurate relations for calculating the optical-field intensity at the center of a spherical particle were obtained in [1] using first-order spherical Riccati–Bessel functions of the first and third kind and their derivatives.

In the present paper, we consider an exact solution of the indicated problem using elementary trigonometric functions and algebraic relations. Approximations of the dependences of the optical-field intensity at the center of a particle on its radius, refractive index, and incident-radiation wavelength. It is shown that at the limit, the obtained solution coincides with the Lorentz formula for local fields in the case of small particles.

Previously [1], it has been shown that at the center of a spherical particle, the optical-field intensity I_{i0} normalized to the incident-wave intensity has the form

$$I_{i0} = E_0^{-2}|C|^2, \tag{1}$$

where

$$C = im/[\xi_1(\rho)\psi_1'(m\rho) - m\xi_1'(\rho)\psi_1(m\rho)]; \tag{2}$$

$$\psi_1(m\rho) = \frac{\sin(m\rho)}{m\rho} - \cos(m\rho), \qquad \psi_1'(m\rho) = -\sin(m\rho)\Big(\frac{1}{(m\rho)^2} - 1\Big) + \frac{\cos(m\rho)}{m\rho},$$
$$\xi_1(\rho) = -(1 - i/\rho)\exp(-i\rho), \qquad \xi_1'(\rho) = -(i/\rho^2 - 1/\rho - i)\exp(-i\rho), \tag{3}$$

$m = n - i\text{æ}$ is the complex refractive index of the material of the spherical particle, $\rho = 2\pi a/\lambda$ is the diffraction parameter of the particle, a is the radius of the particle, λ is the wavelength of the radiation incident on the particle, $\psi(z)$, $\xi(z)$, $\psi'(z)$, and $\xi'(z)$ are first-order spherical Riccati–Bessel functions of the first and third kind and their derivatives.

Substituting (3) into (2) and collecting terms, we obtain

$$C = im/[C_1\sin(\rho m) + C_2\cos(\rho m)]; \tag{4}$$

$$C_1 = -1 + \frac{1/m^2 - 1}{\rho^2} + i\,\frac{1 - 1/m^2}{\rho^3}, \qquad C_2 = im - \frac{1 - i/\rho}{m\rho} + im\,\frac{1 - 1/\rho}{\rho}. \tag{5}$$

Formula (1) with coefficients (4) and (5) yields the exact solution for the optical-field intensity at the center of particles of any radius without restrictions on values of the complex refractive index of the particle material and incident laser radiation wavelengths.

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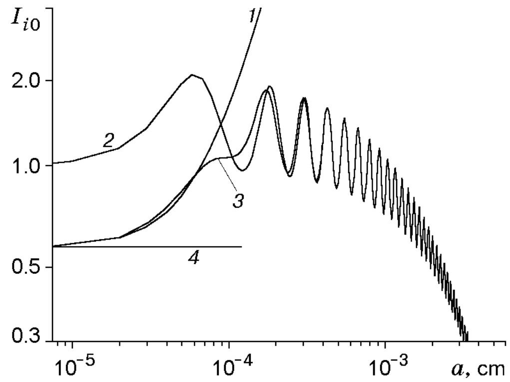

Fig. 1. Relative optical field from radiation of wavelength 3.4483 μm at the center of water particles ($n = 1.4 - 0.0124i$): curve 1 is the approximation (9), (10) for small particles, curve 2 is the approximation (1), (6) for large particles, curve 3 refer to calculations using Mie theory near the center of the particle using formulas (1), (4), and (5), and curve 4 refer to calculations of the optical field in the volume of a small particle by formulas (1) and (7).

To validate the relation obtained, calculations of optical-field intensity were performed using Mie theory for a point at a distance of less than 0.1 nm from the center. It turned out that for this small distance from the center, Mie theory can be employed to calculate the electromagnetic-field components without the risk of occurrence of an indeterminate form of the 0/0 type. Apparently, displacement of the calculation point for a distance of 0.1 nm from the center does not lead to a change in optical-field intensity.

Figure 1 shows the solution obtained from formulas (1), (4), and (5) (curve 3). It should be noted that calculations by Mie theory at the point at 10^{-8} cm from the center are also described by curve 3. The results of calculations using Mie theory and formulas (1), (4), and (5) were compared for aerosol particles of various materials (beryllium oxide, nitromethane, ethanol, gold, alumina, quartz, silver, chlorophyll, and oil) over a broad range of sizes (from several nanometers to hundreds of micrometers) for various radiation wavelengths (from the ultraviolet spectrum to the far infrared region). In all cases, the results of calculations by formulas (1), (4), and (5) agree with calculations using the Mie theory to four-place accuracy.

To obtain an approximation for the optical-field intensity at the center of large particles, in expressions (5), we retain only the first terms ($C_1 = -1$ and $C_2 = im$), i.e., discard terms $1/\rho \ll 1$. Then, Eq. (4) becomes

$$C = im/[-\sin(\rho m) + im\cos(\rho m)]. \tag{6}$$

Expression (1) with coefficient (6) is an adequate approximation of the optical-field intensity at the center of a large particle (for particle radii larger than the wavelength). In Fig. 1, this approximation is shown by curve 2, which coincides with the results of calculations using Mie theory for large particles.

The approximation for small particles is obtained if in (3), we retain terms with $1/\rho \gg 1$:

$$\psi_1(m\rho) = \frac{(m\rho)^2}{3}, \quad \psi_1'(m\rho) = \frac{2m\rho}{3}, \quad \xi_1(\rho) = \frac{i}{\rho}\exp(-i\rho), \quad \xi_1'(\rho) = -\frac{i}{\rho^2}\exp(-i\rho).$$

Then, expression (2) becomes

$$C = 3/(m^2 + 2). \tag{7}$$

The relative intensity at the center of a small particle calculated from (1) and (7) is shown in Fig. 1 by curve 4.

The absorption cross section of the particle σ_p is determined as the product of the radiation intensity inside the particle (the intensity is assumed to be constant with passage from one point to another), the volume of the particle V_p, and the absorption constant of the particle material $\alpha_p = 4\pi n æ/\lambda$ [2]:

$$\sigma_p = I_{i0}\alpha_p V_p = \left(\frac{3}{m^2 + 2}\right)^2 \frac{4\pi n æ}{\lambda} V_p = \frac{36\pi n æ}{(m^2 + 2)^2}\,\frac{V_p}{\lambda}. \tag{8}$$

Formula (8) of the radiation absorption cross section for a particle whose size is much less than the wavelength, obtained from relations (1), (4), and (5), is similar to the formula obtained in [3, p. 86] for small particles.

The approximation of the field at the center of a small particle $\rho|m-1| \ll 1$ can also be found from the formulas for the efficiency of radiation absorption by a particle [4]. For this, we use the relation [4]

$$I_{i0} = 3Q_p/(4\alpha_p a), \tag{9}$$

where $Q_p = Q_e - Q_s$ is the laser radiation absorption efficiency and Q_e and Q_s are the relative efficiencies of attenuation and scattering. For the calculations, we use the following relations for Q_e and Q_s [2]:

$$\begin{gathered} Q_e = 4\rho \operatorname{Im}\Big\{\frac{m^2-1}{m^2+2}\Big[1+\frac{\rho^2}{15}\,\frac{m^2-1}{m^2+2}\,\frac{m^4+27m^2+38}{2m^2+3}\Big]\Big\} + \frac{8}{3}\,\rho^4 \operatorname{Re}\Big\{\Big(\frac{m^2-1}{m^2+2}\Big)^2\Big\}, \\ Q_s = (8\rho^4/3)|(m^2-1)/(m^2+2)|^2. \end{gathered} \tag{10}$$

In Fig. 1, curve 1 is the approximation for small particles calculated from formulas (9) and (10). It is evident that this approximation agrees well with results of calculations by relations (1), (4), and (5) for particles of radius less than 1 μm.

In conclusion, it should be noted that for $\rho|m-1| \ll 10^{-2}$, calculations by formulas (1)–(5), (9), and (10) should be performed to double precision (for example, Real*8, Complex*16). This guarantees high accuracy of calculations irrespective of the initial data. In calculations with low-precision representation of a number, for example, Real*4, random outliers comparable to the solution arise for small particle sizes.

In [5, 6], it is shown that in the volume of a small aerosol particle in a laser radiation field, the optical-field intensity can vary over a wide range. Some part of the particle material is heated to a temperature far exceeding its boiling point while most of the particle remains rather cold. In this case, to estimate the thermal explosion of the entire particle, one need to determine the characteristic intensity of the optical field for most of the particle material. The magnitude of the optical field at the center of the particle is an adequate estimate of this parameter. Thus, the results obtained makes is possible to estimate the probability of thermal explosion of most of the particle material. Such estimates are important for the development of aerosol mass spectrometry, which uses powerful pulse lasers for evaporation of drops in an ionization chamber [7].

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