ISSN 0027-1349, Moscow University Physics Bulletin, 2025, Vol. 80, No. 3, pp. 537–544. © Allerton Press, Inc., 2025.
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OPTICS AND SPECTROSCOPY. LASER PHYSICS

Surface Perturbation Theory in the Problem of Light Elastic Scattering on Microparticles

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Received January 7, 2025; revised February 10, 2025; accepted February 18, 2025

Abstract—Using the method of perturbation theory, the problem of light scattering by particles of arbitrary axisymmetric shape has been solved. The proposed approach makes it possible to consider substantial deformations by decomposing the total deformation into smaller ones. The issues of convergence, applicability limits and conditions are discussed; a comparison with an alternative computational method is presented.

Keywords: Mie theory, the T-matrix method, light scattering, perturbation theory

DOI: 10.3103/S0027134925700584

INTRODUCTION

The problem of elastic light scattering by particles has a wide range of applications in science and technology. There exist numerous approaches and approximations for its solution. If the particle size greatly exceeds the wavelength, the laws of geometrical optics are used [1]. In the opposite case, it is necessary to solve Maxwell's equations, that is, to apply the laws of wave optics. The literature presents a number of methods for solving this problem, the choice of which is determined by the conditions and the required accuracy. Among analytical methods, one can distinguish the point matching method [2], the T-matrix method or the extended boundary condition method (EBCM) [3, 4], and the method of separation of variables (which in the case of a sphere reduces to Mie theory) [5]. Numerical methods include the method of moments [6], the finite-difference time-domain method [7], the volume integral equation method [8], and the finite element method [9].

Analytical methods provide high accuracy and require less computational cost, but their application is generally limited to simple geometries, such as spheres and ellipsoids.

The work [10] presents a method for calculating light scattering by a particle of complex shape based on perturbation theory of the surface relative to a spherical one. However, this method is significantly limited by the magnitude of the surface perturbation, as has been repeatedly emphasized in the literature [11, 12]. To overcome this limitation, the initial deformation can be decomposed into a set of small perturbations. Nevertheless, in this case it is required to modify the theory for an arbitrary initial surface rather than only a spherical one. This approach was first applied in [13] for the case of scattering of a plane wave. In the present work, scattering is considered for an arbitrary wave shape.

The content of this work is organized as follows. Sections 1–3 present the main formulae and principles of the method; limits and conditions of applicability are discussed. Section 4 discusses comparison with the EBCM method [3]; problems are indicated for which we recommend using our method.

1. PROBLEM STATEMENT

Let the time dependence of the electromagnetic field be given by $\exp(-i\omega t)$, where ω is the angular frequency of light. Then the spatial dependence of the field satisfies the vector Helmholtz equation:

$$\Delta\mathbf{E} + n_{\text{glob}}^2 k^2 \mathbf{E} = 0, \qquad (1)$$

which must be solved in two domains—inside the particle (refractive index $n_{\text{glob}} = n_{\text{refr}}$), and outside (we assume the refractive index of the surrounding medium is equal to $n_{\text{glob}} = 1$), $k = \omega/c$, c is the speed of light. In our problem, it is convenient to consider a spherical coordinate system, in which the fundamental solutions of (1) are vector spherical harmonics:

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$$\mathbf{M}_{\pm mn} = z_n(\rho)\mathbf{m}_{\pm mn},$$
$$\mathbf{N}_{\pm mn} = \frac{z_n(\rho)}{\rho}\mathbf{p}_{\pm mn} + \frac{[\rho z_n(\rho)]'}{\rho}\mathbf{n}_{\pm mn}, \quad (2)$$

where

$$\mathbf{m}_{\pm mn} = \mp\pi_{mn}\begin{bmatrix}\sin m\varphi\\ \cos m\varphi\end{bmatrix}\mathbf{e}_\theta - \tau_{mn}\begin{bmatrix}\cos m\varphi\\ \sin m\varphi\end{bmatrix}\mathbf{e}_\varphi,$$
$$\mathbf{n}_{\pm mn} = \tau_{mn}\begin{bmatrix}\cos m\varphi\\ \sin m\varphi\end{bmatrix}\mathbf{e}_\theta \mp \pi_{mn}\begin{bmatrix}\sin m\varphi\\ \cos m\varphi\end{bmatrix}\mathbf{e}_\varphi,$$
$$\mathbf{p}_{\pm mn} = n(n+1)P_n^m(\cos\theta)\begin{bmatrix}\cos m\varphi\\ \sin m\varphi\end{bmatrix}\mathbf{e}_r. \quad (3)$$

Here $\pi_{mn} = \frac{m}{\sin\theta}P_n^m(\cos\theta)$, $\tau_{mn} = \frac{d}{d\theta}P_n^m(\cos\theta)$, and $P_n^m(\cos\theta)$ are the associated Legendre polynomials, (r,θ,ϕ) are spherical coordinates, ($\mathbf{e}_r$, $\mathbf{e}_\theta$, $\mathbf{e}_\varphi$) are the corresponding unit vectors, $z_n(\rho)$—spherical Bessel functions, $\rho = kr$ is the dimensionless radius (inside the particle it is multiplied by the refractive index n_{refr}).

Let the initial shape of the particle σ_0 be described by the equation $r = r_0 f_0(\theta)$. In order to construct perturbation theory for this surface, it is necessary to know the solution for an arbitrary field on the original surface σ_0. Moreover, as will become clear from the discussion below, it is necessary to know the solution under the condition of independence of the fields $\mathbf{E}$ and $\mathbf{H}$, whereas in the standard light scattering problem it is assumed that these fields are related through Maxwell's equations.

Let us consider the scattering of the field $\mathbf{E}^{\text{inc}}$ by a particle with refractive index n_{refr} and magnetic permeability μ, with a surface shape σ_1 defined by the following equation:

$$r = r_0\left(f_0(\theta) + \varepsilon f_1(\theta)\right). \quad (4)$$

Due to the completeness of the system of functions (2), an arbitrary field $\mathbf{E}^{\text{inc}}$ can be expanded in a series of $\mathbf{M}_{\pm mn}$ and $\mathbf{N}_{\pm mn}$ [14]. By virtue of the axial symmetry of the particle (4), it is sufficient to consider only the TM mode, so that

$$\mathbf{E}^{\text{inc}} = \sum_{n=1}^{\infty}\sum_{m=0}^{n}\left(e_{+mn}\mathbf{N}^{(1)}_{+mn} + f_{-mn}\mathbf{M}^{(1)}_{-mn}\right), \quad (5)$$

where the superscript (1) denotes the choice of the spherical Bessel function of the first kind, $z_n(\rho) = j_n(\rho)$. The solution for the TE mode can be obtained from the solution for the TM mode [15]. The scattered field $\mathbf{E}^{\text{sca}}$ and the internal field $\mathbf{E}^{\text{int}}$ can be represented as series:

$$\mathbf{E}^{\text{sca}} = \sum_{n=1}^{\infty}\sum_{m=0}^{n}\left(a_{+mn}\mathbf{N}^{(3)}_{+mn} + b_{-mn}\mathbf{M}^{(3)}_{-mn}\right),$$
$$\mathbf{E}^{\text{int}} = \sum_{n=1}^{\infty}\sum_{m=0}^{n}\left(d_{+mn}\mathbf{N}^{(1)}_{+mn} + c_{-mn}\mathbf{M}^{(1)}_{-mn}\right), \quad (6)$$

where the superscript (3) denotes the choice of the spherical Hankel function of the first kind, $z_n(\rho) = h_n^{(1)}(\rho)$.

The unknown coefficients (a,b,c,d) in Eq. (6) are determined from the boundary conditions on the surface of the particle σ_1, which require continuity of the tangential components of the electric and magnetic fields:

$$\left(f_0 + \varepsilon f_1\right)\mathbf{E}^{\text{out}}_\tau + \left(f_{0\theta} + \varepsilon f_{1\theta}\right)E^{\text{out}}_r\mathbf{e}_\theta$$
$$= \left(f_0 + \varepsilon f_1\right)\mathbf{E}^{\text{int}}_\tau + \left(f_{0\theta} + \varepsilon f_{1\theta}\right)E^{\text{int}}_r\mathbf{e}_\theta,$$
$$\left(f_0 + \varepsilon f_1\right)\mathbf{H}^{\text{out}}_\tau + \left(f_{0\theta} + \varepsilon f_{1\theta}\right)H^{\text{out}}_r\mathbf{e}_\theta$$
$$= \left(f_0 + \varepsilon f_1\right)\mathbf{H}^{\text{int}}_\tau + \left(f_{0\theta} + \varepsilon f_{1\theta}\right)H^{\text{int}}_r\mathbf{e}_\theta, \quad (7)$$

where $f_{i\theta} \equiv \frac{\partial f_i}{\partial\theta}$ and $\mathbf{E}_\tau \equiv E_\varphi\mathbf{e}_\varphi + E_\theta\mathbf{e}_\theta$, $\mathbf{E}^{\text{out}} = \mathbf{E}^{\text{inc}} + \mathbf{E}^{\text{sca}}$, analogously for $\mathbf{H}$. Substituting (6) into (7), we obtain:

$$\sum_{mn}\Big[\left(b_{-mn}\beta_n^0 - \kappa c_{-mn}\alpha_n^0\right)\mathbf{m}_{-mn} + \left(a_{+mn}\beta_n^1 - \kappa d_{+mn}\alpha_n^1\right)\mathbf{n}_{+mn}$$
$$+ \mathbf{e}_\theta\rho_0 f_{0\theta}\left(a_{+mn}\eta_n^0 - \kappa d_{+mn}\sigma_n^0\right)p_{+mn}\Big]\Big|_{r\in\sigma_1}$$
$$= -\rho_0\left(f_0 + \varepsilon f_1\right)\mathbf{E}^{\text{inc}}_\tau - \rho_0\left(f_{0\theta} + \varepsilon f_{1\theta}\right)\mathbf{e}_\theta E^{\text{inc}}_r\Big|_{r\in\sigma_1},$$
$$\sum_{mn}\Big[\chi_1\left(a_{+mn}\beta_n^0 - \chi_2\kappa c_{+mn}\alpha_n^0\right)\mathbf{m}_{+mn} + \left(\chi_1 b_{-mn}\beta_n^1 - \chi_2\kappa c_{-mn}\alpha_n^1\right)\mathbf{n}_{-mn}$$

$$+\mathbf{e}_\theta\rho_0 f_{0\theta}\left(\chi_1 b_{-mn}\eta_n^0-\chi_2\kappa c_{-mn}\sigma_n^0\right)p_{-mn}\Big]\Big|_{r\in\sigma_1}$$
$$=-\rho_0\left(f_0+\varepsilon f_1\right)\mathbf{H}_\tau^{\text{inc}}-\rho_0\left(f_{0\theta}+\varepsilon f_{1\theta}\right)\mathbf{e}_\theta H_r^{\text{inc}}\Big|_{r\in\sigma_1}, \quad (8)$$

where $\rho_0=kr_0$, $\kappa=1/n_{\text{refr}}$, $\chi_1=-i$, $\chi_2=-i\frac{n_{\text{refr}}}{\mu}$. The notations for α,β,σ, and η are the same as in [10, 13]; see also Appendix.

2. GENERALIZED SURFACE PERTURBATION THEORY

We seek a solution to system (8) in the form of a series of the small parameter ε:

$$(a,b,c,d)_{mn}=\sum_{p=0}^{\infty}(a,b,c,d)_{mn}^p\varepsilon^p. \quad (9)$$

To construct the perturbation theory, Eqs. (8) should be expanded in a series of ε taking into account (9). The equations for determining the unknowns are obtained by equating the coefficients at powers of ε^p.

Some key remarks should be made. In [10], all terms related to the incident field are also expanded in a series of ε. However, this is not necessary, since these quantities are known and can be computed as independent of ε. This approach not only simplifies the formulae but also allows constructing the solution in a more general form.

More detailed derivations are presented in Appendix, from which it follows that the expansion (8) can be written in the form:

$$\sum_{mn}\Big[\left(b_{-mn}^l\beta_n^0-\kappa c_{-mn}^l\alpha_n^0\right)\mathbf{m}_{-mn}+\left(a_{+mn}^l\beta_n^1-\kappa d_{+mn}^l\alpha_n^1\right)\mathbf{n}_{+mn}$$
$$+\mathbf{e}_\theta\rho_0 f_{0\theta}\left(a_{+mn}^l\eta_n^0-\kappa d_{+mn}^l\sigma_n^0\right)p_{+mn}\Big]\Big|_{r\in\sigma_0}=\mathbf{S}_l,$$
$$\sum_{mn}\Big[\left(\chi_1 a_{+mn}^l\beta_n^0-\chi_2\kappa d_{+mn}^l\alpha_n^0\right)\mathbf{m}_{+mn}+\left(\chi_1 b_{-mn}^l\beta_n^1-\chi_2\kappa c_{-mn}^l\alpha_n^1\right)\mathbf{n}_{-mn}$$
$$+\mathbf{e}_\theta\rho_0 f_{0\theta}\left(\chi_1 b_{-mn}^l\eta_n^0-\chi_2\kappa c_{-mn}^l\sigma_n^0\right)p_{-mn}\Big]\Big|_{r\in\sigma_0}=\mathbf{T}_l, \quad (10)$$

where $l=0,1,2,3..$, the quantities $\mathbf{S}_l$, $\mathbf{T}_l$ are computed as follows for $l=0$:

$$\mathbf{S}_0=-\rho_0\left(f_0+\varepsilon f_1\right)\mathbf{E}_\tau^{\text{inc}}-\rho_0\left(f_{0\theta}+\varepsilon f_{1\theta}\right)\mathbf{e}_\theta E_r^{\text{inc}}\Big|_{r\in\sigma_1},$$
$$\mathbf{T}_0=-\rho_0\left(f_0+\varepsilon f_1\right)\mathbf{H}_\tau^{\text{inc}}-\rho_0\left(f_{0\theta}+\varepsilon f_{1\theta}\right)\mathbf{e}_\theta H_r^{\text{inc}}\Big|_{r\in\sigma_1}, \quad (11)$$

for $l>0$:

$$\mathbf{S}_l=\sum_{q=0}^{l-1}\sum_{mn}\frac{f_1^{l-q}}{(l-q)!}\Big[\left(\kappa c_{-mn}^q\alpha_n^{l-q}\rho_{20}^{l-q}-b_{-mn}^q\beta_n^{l-q}\rho_0^{l-q}\right)\mathbf{m}_{-mn}$$
$$+\left(\kappa d_{+mn}^q\alpha_n^{l-q+1}\rho_{20}^{l-q}-a_{+mn}^q\beta_n^{l-q+1}\rho_0^{l-q}\right)\mathbf{n}_{+mn}$$
$$+\left(d_{+mn}^q\sigma_n^{l-q}\rho_{20}^{l-q}-a_{+mn}^q\eta_n^{l-q}\rho_0^{l-q}\right)f_{0\theta}\rho_0\mathbf{e}_\theta p_{+mn}$$
$$+\Big(\quad d_{+mn}^q\sigma_n^{l-q-1}\rho_{20}^{l-q-1}-\quad a_{+mn}^q\eta_n^{l-q-1}\rho_0^{l-q-1}\Big)f_{1\theta}\rho_0\frac{l-q}{f_1}\mathbf{e}_\theta p_{+mn}\Big]\Big|_{r\in\sigma_0},$$

$$\mathbf{T}_l = \sum_{q=0}^{l-1}\sum_{mn}\frac{f_1^{l-q}}{(l-q)!}\Big[\Big(\kappa\chi_2 d_{+mn}^q\alpha_n^{l-q}\rho_{20}^{l-q} - \chi_1 a_{+mn}^q\beta_n^{l-q}\rho_0^{l-q}\Big)\mathbf{m}_{+mn} + \Big(\kappa\chi_2 c_{-mn}^q\alpha_n^{l-q+1}\rho_{20}^{l-q} - \chi_1 b_{-mn}^q\beta_n^{l-q+1}\rho_0^{l-q}\Big)\mathbf{n}_{-mn} + \Big(\chi_2 c_{-mn}^q\sigma_n^{l-q}\rho_{20}^{l-q} - \chi_1 b_{-mn}^q\eta_n^{l-q}\rho_0^{l-q}\Big) f_{0\theta}\rho_0\mathbf{e}_\theta p_{-mn} + \Big(\chi_2 c_{-mn}^q\sigma_n^{l-q-1}\rho_{20}^{l-q-1} - \chi_1 b_{-mn}^q\eta_n^{l-q-1}\rho_0^{l-q-1}\Big) f_{1\theta}\rho_0\frac{l-q}{f_1}\mathbf{e}_\theta p_{-mn}\Big]\Big|_{r\in\sigma_0}, \tag{12}$$

$\rho_{20} = n_{\text{refr}}\rho_0$. Comparing conditions (8) and (10), one can observe that the problem reduces to an analogous one, but on the unperturbed surface. As assumed at the beginning of the exposition, the solution on the surface σ_0 is known for any incident field. Moreover, this solution must be expressed under the assumption of independence of $\mathbf{S}_l$, $\mathbf{T}_l$, since the relation between $\mathbf{S}_l$ and $\mathbf{T}_l$ in Eqs. (10) is not known in advance. This is necessary for several reasons: first, this relation depends on the perturbation f_1; second, it is different for different orders l. Thus, although all quantities for $\mathbf{S}_l$ and $\mathbf{T}_l$ depend linearly on the expansion coefficients e_{+nm} and f_{-nm}, in constructing the solution for an arbitrary perturbation f_1 it is convenient to have a solution to Eqs. (10) on the initial surface σ_0 for independent $\mathbf{S}$ and $\mathbf{T}$. This solution is readily obtained in the case of a sphere. In this case, Eqs. (10) take the form:

$$\sum_{mn}\big[(b_{-mn}\beta_n^0 - \kappa c_{-mn}\alpha_n^0)\mathbf{m}_{-mn} + (a_{+mn}\beta_n^1 - \kappa d_{+mn}\alpha_n^1)\mathbf{n}_{+mn}\big]\big|_{r=r_0} = \mathbf{S},$$
$$\sum_{mn}\big[(\chi_1 a_{+mn}\beta_n^0 - \chi_2\kappa d_{+mn}\alpha_n^0)\mathbf{m}_{+mn} + (\chi_1 b_{-mn}\beta_n^1 - \chi_2\kappa c_{-mn}\alpha_n^1)\mathbf{n}_{-mn}\big]\big|_{r=r_0} = \mathbf{T}. \tag{13}$$

Taking into account the orthogonality and completeness of the system of functions $\mathbf{m}_{\pm mn}$ and $\mathbf{n}_{\pm mn}$, expressions (13) can be written in the form of a system of linear equations:

$$b_{-mn}\rho_0 h_n^{(1)}(\rho_0) - \kappa c_{-mn}n_{\text{refr}}\rho_0 j_n(n_{\text{refr}}\rho_0) = \langle\mathbf{S},\mathbf{m}_{-mn}\rangle,$$
$$a_{+mn}[\rho_0 h_n^{(1)}(\rho_0)]' - \kappa d_{+mn}[n_{\text{refr}}\rho_0 j_n(n_{\text{refr}}\rho_0)]' = \langle\mathbf{S},\mathbf{n}_{+mn}\rangle,$$
$$\chi_1 a_{+mn}\rho_0 h_n^{(1)}(\rho_0) - \chi_2\kappa d_{+mn}n_{\text{refr}}\rho_0 j_n(n_{\text{refr}}\rho_0) = \langle\mathbf{T},\mathbf{m}_{+mn}\rangle,$$
$$\chi_1 b_{-mn}[\rho_0 h_n^{(1)}(\rho_0)]' - \chi_2\kappa c_{-mn}[n_{\text{refr}}\rho_0 j_n(n_{\text{refr}}\rho_0)]' = \langle\mathbf{T},\mathbf{n}_{-mn}\rangle, \tag{14}$$

where the explicit form for α and β has been substituted, $\langle\mathbf{S},\mathbf{m}_{-mn}\rangle \equiv \frac{1}{\xi_{mn}}\int_0^\pi\int_0^{2\pi}(\mathbf{S}\cdot\mathbf{m}_{-mn})\times\sin\theta d\theta d\varphi$, $\xi_{mn} = \frac{2n(n+1)(n+m)!}{(2n+1)(n-m)!}(1+\delta_{m0})\pi$. Analogously for $\langle\mathbf{S},\mathbf{n}_{+mn}\rangle$, $\langle\mathbf{T},\mathbf{m}_{+mn}\rangle$, $\langle\mathbf{T},\mathbf{n}_{-mn}\rangle$. The solution to system (14) is:

$$a_{+mn} = \frac{[n_{\text{refr}}\rho_0 j_n(n_{\text{refr}}\rho_0)]'\langle\mathbf{T},\mathbf{m}_{+mn}\rangle - \chi_2 n_{\text{refr}}\rho_0 j_n(n_{\text{refr}}\rho_0)\langle\mathbf{S},\mathbf{n}_{+mn}\rangle}{\chi_1\rho_0 h_n^{(1)}(\rho_0)[n_{\text{refr}}\rho_0 j_n(n_{\text{refr}}\rho_0)]' - \chi_2 n_{\text{refr}}\rho_0 j_n(n_{\text{refr}}\rho_0)[\rho_0 h_n^{(1)}(\rho_0)]'},$$
$$b_{-mn} = \frac{n_{\text{refr}}\rho_0 j_n(n_{\text{refr}}\rho_0)\langle\mathbf{T},\mathbf{n}_{-mn}\rangle - \chi_2[n_{\text{refr}}\rho_0 j_n(n_{\text{refr}}\rho_0)]'\langle\mathbf{S},\mathbf{m}_{-mn}\rangle}{\chi_1 n_{\text{refr}}\rho_0 j_n(n_{\text{refr}}\rho_0)[\rho_0 h_n^{(1)}(\rho_0)]' - \chi_2\rho_0 h_n^{(1)}(\rho_0)[n_{\text{refr}}\rho_0 j_n(n_{\text{refr}}\rho_0)]'},$$
$$c_{-mn} = \frac{\rho_0 h_n^{(1)}(\rho_0)\langle\mathbf{T},\mathbf{n}_{-mn}\rangle - \chi_1[\rho_0 h_n^{(1)}(\rho_0)]'\langle\mathbf{S},\mathbf{m}_{-mn}\rangle}{\kappa\Big(\chi_1 n_{\text{refr}}\rho_0 j_n(n_{\text{refr}}\rho_0)[\rho_0 h_n^{(1)}(\rho_0)]' - \chi_2\rho_0 h_n^{(1)}(\rho_0)[n_{\text{refr}}\rho_0 j_n(n_{\text{refr}}\rho_0)]'\Big)},$$
$$d_{+mn} = \frac{[\rho_0 h_n^{(1)}(\rho_0)]'\langle\mathbf{T},\mathbf{m}_{+mn}\rangle - \chi_1\rho_0 h_n^{(1)}(\rho_0)\langle\mathbf{S},\mathbf{n}_{+mn}\rangle}{\kappa\Big(\chi_1\rho_0 h_n^{(1)}(\rho_0)[n_{\text{refr}}\rho_0 j_n(n_{\text{refr}}\rho_0)]' - \chi_2 n_{\text{refr}}\rho_0 j_n(n_{\text{refr}}\rho_0)[\rho_0 h_n^{(1)}(\rho_0)]'\Big)}. \tag{15}$$

Formulae (15) can be written in matrix form:

$$\begin{bmatrix} a_{+mn} \\ b_{-mn} \\ c_{-mn} \\ d_{+mn} \end{bmatrix} = \hat{G}_0 \begin{bmatrix} \langle \mathbf{S}, \mathbf{n}_{+mn} \rangle \\ \langle \mathbf{S}, \mathbf{m}_{-mn} \rangle \\ \langle \mathbf{T}, \mathbf{n}_{-mn} \rangle \\ \langle \mathbf{T}, \mathbf{m}_{+mn} \rangle \end{bmatrix}, \qquad (16)$$

where the components of the matrix $\hat{G}_0$ are determined from expressions (15). In this notation, the indices m and n take all possible values. Note that due to the symmetry with respect to the z-axis, formula (16) can be written separately for each of the azimuthal modes m. The matrix $\hat{G}_0$ defines the solution for independent $\mathbf{S}$ and $\mathbf{T}$, which is required for constructing the solution in the case of a surface perturbation.

Knowing the matrix $\hat{G}$ for the initial surface σ_0, one can compute the corresponding matrix $\hat{G}'$ for the perturbed surface σ_1 using the method of perturbation theory. For this purpose, it is necessary to determine the solution of system (10) for all orders l, assuming in (11) that $\mathbf{S}_0 = \mathbf{m}_{mn}$ or $\mathbf{n}_{mn}$, $\mathbf{T}_0 = 0$, or in the case $\mathbf{T}_0 = \mathbf{m}_{mn}$ or $\mathbf{n}_{mn}$, $\mathbf{S}_0 = 0$. Summing the perturbation series (9), we obtain the coefficients $(a, b, c, d)_{mn}$, which will form the corresponding columns in (16) for the new matrix $\hat{G}'$. This solution will describe the scattering of a field for which the right-hand side of Eqs. (8) is equal to the corresponding harmonic $\mathbf{m}_{\pm mn}$ or $\mathbf{n}_{\pm mn}$.

Successive application of perturbation theory by the method described above allows one to achieve substantial deformations relative to the original spherical surface, which are not possible with a single application of perturbation theory.

3. CONDITIONS OF APPLICABILITY

The magnitude of the perturbation is determined by the convergence of the series (9), the criterion for which is the smallness of the perturbation. However, it is necessary to clarify what is meant by the "smallness" of a continuous quantity. It is not difficult to show that the simple condition $|\varepsilon f_1(\theta)| < 1$ is insufficient for convergence of the series (9), since it is also necessary to bound the derivative $|\varepsilon f'_{1\theta}(\theta)| < 1$, see [11]. This gives rise to the need to characterize the smallness of deformations in a universal way. For this purpose, we will write f_1 in the form of a trigonometric series:

$$f_1(\theta) = x_0 + \sum_{j=1} \big(x_j \cos j\theta + y_j \sin j\theta\big). \qquad (17)$$

The smallness of the perturbation is conveniently defined by the quantity

$$\|f_1\| = |x_0| + \sum_{j=1} j\big(|x_j| + |y_j|\big). \qquad (18)$$

In this case, the smallness of the quantity $\varepsilon\|f_1\| < 1$ guarantees both conditions $|\varepsilon f_1(\theta)|$, $|\varepsilon f'_{1\theta}(\theta)| < 1$. The choice of intermediate deformations between the initial and final shapes also has a significant effect on the convergence of the result. It is evident that such a transition can be performed in many ways. Our calculations show that the choice of the path of intermediate deformations affects the convergence of the result even under identical constraints on the perturbation magnitude (18).

From a physical point of view, the reason for the limitation on the magnitude of the deformation lies in the eigenmodes of the particle. This statement is easy to explain in the case of deformation of the spherical surface by a constant value. In this case, expressions (15) should transform into themselves, but for a different particle radius. Thus, the series (9) represents a Taylor series with respect to the parameter ρ_0. The radius of convergence is determined by the zeros in the denominators in (15); the corresponding values of the size parameter lie in the complex plane [11] and limit the radius of convergence of the series (9), despite the fact that expressions (15) have no singularities on the real axis. In the more general case, determining the eigenmodes represents a separate labor-intensive task [11, 12]. Thus, the optimal deformation path is the one that lies at the maximum distance from the eigenmodes. This explains the dependence of the result on the choice of the deformation path.

Another factor limiting the applicability of the presented method is the inevitable accumulation of numerical error in the calculation. Any numerical computation is carried out for a limited number of modes $\mathbf{m}_{mn}$ and $\mathbf{n}_{mn}$ in the expansions (5) and (6). Let this number be denoted as $N_{\max}$. When constructing the series in perturbation theory in the case of a nonconstant perturbation, the functions $\mathbf{S}$, $\mathbf{T}$ may contain a greater number of modes than are included in the computation, due to which the modes with index $n > N_{\max}$ are not taken into account in the solution, which leads to the accumulation of error.

4. STABILITY ANALYSIS IN THE NEAR FIELD, COMPARISON WITH THE T-MATRIX METHOD

The literature contains a number of methods for solving light scattering problems on structures of various shapes [16]. Among them, the method most closely related in content is the extended boundary

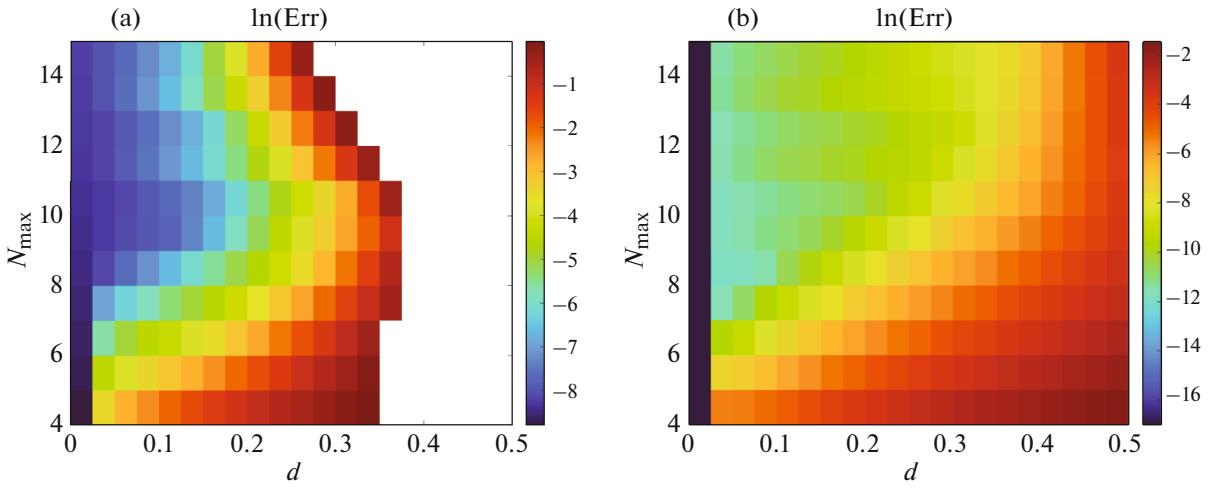

Fig. 1. Comparison of accuracy and stability of computations using the EBCM method (a) and perturbation theory (b) as a function of perturbation magnitude d and maximum number of modes N_{max}. The absence of part of the data in (a) indicates divergence of the method at Err > 1.

condition method (EBCM) [17, 18]. In this section, we present a comparison between our proposed method and EBCM. For this purpose, we performed calculations for a Chebyshev particle described by the equation

$$kr = 3(1 + d\cos\varphi), \tag{19}$$

where the parameter d characterizes the curvature of the particle. In Fig. 1, an accuracy estimate of the two methods is shown as a function of d. As a measure of accuracy, we verified the boundary conditions and calculated the error:

$$\mathrm{Err} = \frac{\iint\left|[\mathbf{n},(\mathbf{H}^2-\mathbf{H}^1)]\right|d\Omega}{\iint\left|[\mathbf{n},\mathbf{H}^{\mathrm{inc}}]\right|d\Omega} + \frac{\iint\left|[\mathbf{n},(\mathbf{E}^2-\mathbf{E}^1)]\right|d\Omega}{\iint\left|[\mathbf{n},\mathbf{E}^{\mathrm{inc}}]\right|d\Omega}.$$

Note that the presented estimate characterizes the accuracy of the solution in the near field, which, in the case of EBCM, is lower than in the far field. For $d > 0.35$ EBCM exhibits clear divergence, which is associated with the numerical instability of the method [18]. Our method demonstrates slightly greater stability and works up to $d < 0.5$, but more importantly, it remains stable with increasing maximum number of modes in the expansions.

For sufficiently large amplitudes ($d > 0.1$), the computation time is lower for EBCM than when using the perturbation theory method, since multiple applications of the theory are required. Thus, our method is most suitable for sufficiently complex geometries. Another area of application is optimization problems, where it is necessary to perform multiple computations for particles with similar geometry and gradual shape variation. In this case, perturbation theory can be applied to previously computed cases with similar geometry, which does not require repeated application of the perturbation theory. In conclusion, we note that other methods listed in the introduction may also exhibit greater stability compared to EBCM. For this reason, the presented comparison does not imply that our proposed method will have an advantage over all others.

CONCLUSIONS

This work presents a method for computing light scattering by particles of complex shape within the framework of surface perturbation theory. It is shown that the method exhibits greater numerical stability compared to EBCM. The analysis was carried out for deformations of type (19), but our experience with these methods shows that this trend persists in other cases as well. It should be noted that there are cases in which the presented method is less efficient, particularly for strongly elongated elliptical particles. For this case, several methods exist for optimizing EBCM [19, 20], which provide higher accuracy and stability.

FUNDING

This study was carried out within the framework of the state assignment of Lomonosov Moscow State University and was also supported by a grant from the Foundation for the Advancement of Theoretical Physics and Mathematics “BASIS” (grant no. 23-1-1-61).

CONFLICT OF INTEREST

The authors of this work declare that they have no conflicts of interest.

APPENDIX

PERTURBATION THEORY SERIES

Let us substitute the expansion (9) into the boundary conditions (8). To do this, we expand the following functions into a Taylor series:

$$\rho h_n^{(1)}(\rho)\big|_{\sigma_1} = \sum_{p=0}^{\infty} \varepsilon^p \frac{\beta_n^p}{p!} \rho_0^p f_1^p,$$

$$\beta_n^p(\theta) = \frac{d^p}{d\rho^p}\left[\rho h_n^{(1)}(\rho)\right]\Big|_{\rho=\rho_0 f_0(\theta)}, \qquad \text{(A.1.1)}$$

$$n_{\text{refr}}\rho j_n(n_{\text{refr}}\rho)\big|_{\sigma_1} = \sum_{p=0}^{\infty} \varepsilon^p \frac{\alpha_n^p}{p!} (n_{\text{refr}}\rho_0)^p f_1^p,$$

$$\alpha_n^p(\theta) = \frac{d^p}{d\rho^p}\left[\rho j_n(\rho)\right]\Big|_{\rho=n_{\text{refr}}\rho_0 f_0(\theta)}, \qquad \text{(A.1.2)}$$

$$\frac{h_n^{(1)}(\rho)}{\rho}\Big|_{\sigma_1} = \sum_{p=0}^{\infty} \varepsilon^p \frac{\eta_n^p}{p!} \rho_0^p f_1^p,$$

$$\eta_n^p(\theta) = \frac{d^p}{d\rho^p}\left[\frac{h_n^{(1)}(\rho)}{\rho}\right]\Big|_{\rho=\rho_0 f_0(\theta)}, \qquad \text{(A.1.3)}$$

$$\frac{j_n(n_{\text{refr}}\rho)}{n_{\text{refr}}\rho}\Big|_{\sigma_1} = \sum_{p=0}^{\infty} \varepsilon^p \frac{\sigma_n^p}{p!} (n_{\text{refr}}\rho_0)^p f_1^p,$$

$$\sigma_n^p(\theta) = \frac{d^p}{d\rho^p}\left[\frac{j_n(\rho)}{\rho}\right]\Big|_{\rho=n_{\text{refr}}\rho_0 f_0(\theta)}. \qquad \text{(A.1.4)}$$

Using the formula $\left(\sum_{p=0}^{\infty} \varepsilon^p a^p\right)\left(\sum_{p=0}^{\infty} \varepsilon^p b^p\right) = \sum_{p=0}^{\infty} \varepsilon^p \sum_{q=0}^{p} a^q b^{p-q}$, we obtain:

$$\begin{aligned}
&\sum_{p=0}^{\infty} \varepsilon^p \sum_{mn} \sum_{q=0}^{p} \frac{f_1^{p-q}}{(p-q)!} \Big[\left(b_{-mn}^q \beta_n^{p-q} \rho_0^{p-q} - \kappa c_{-mn}^q \alpha_n^{p-q} \rho_{20}^{p-q} \right) \mathbf{m}_{-mn} \\
&\quad + \left(a_{+mn}^q \beta_n^{p-q+1} \rho_0^{p-q} - \kappa d_{+mn}^q \alpha_n^{p-q+1} \rho_{20}^{p-q} \right) \mathbf{n}_{+mn} \\
&\quad + \left(a_{+mn}^q \eta_n^{p-q} \rho_0^{p-q} - d_{+mn}^q \sigma_n^{p-q} \rho_{20}^{p-q} \right) f_{0\theta} \rho_0 \mathbf{e}_\theta p_{+mn} \\
&\quad + \left(a_{+mn}^q \eta_n^{p-q-1} \rho_0^{p-q-1} d_{+mn}^q \sigma_n^{p-q-1} \rho_{20}^{p-q-1} \right) f_{1\theta} \rho_0 \frac{p-q}{f_1} \mathbf{e}_\theta p_{+mn} \Big] \Big|_{r\in\sigma_0} \\
&\quad = -\rho_0 \left(f_0 + \varepsilon f_1\right) \mathbf{E}_\tau^{\text{inc}} - \rho_0 \left(f_{0\theta} + \varepsilon f_{1\theta}\right) \mathbf{e}_\theta E_r^{\text{inc}} \Big|_{r\in\sigma_1}. \qquad \text{(A.2)}
\end{aligned}$$

Now that we have expanded the boundary conditions into a series of powers of the small parameter ε, we require that the equality holds for each term of this series separately. To this end, let us consider a certain lth term of the series $\sum_p$, where $l > 0$. In this case, since the incident field is given, it is convenient to assign it to the quantity of zeroth order in smallness, see (11)

$$\begin{aligned}
&\sum_{mn} \sum_{q=0}^{l} \frac{f_1^{l-q}}{(l-q)!} \Big[\left(b_{-mn}^q \beta_n^{l-q} \rho_0^{l-q} - \kappa c_{-mn}^q \alpha_n^{l-q} \rho_{20}^{l-q} \right) \mathbf{m}_{-mn} \\
&\quad + \left(a_{+mn}^q \beta_n^{l-q+1} \rho_0^{l-q} - \kappa d_{+mn}^q \alpha_n^{l-q+1} \rho_{20}^{l-q} \right) \mathbf{n}_{+mn} \\
&\quad + \left(a_{+mn}^q \eta_n^{l-q} \rho_0^{l-q} - d_{+mn}^q \sigma_n^{l-q} \rho_{20}^{l-q} \right) f_{0\theta} \rho_0 \mathbf{e}_\theta p_{+mn} \\
&\quad + \left(a_{+mn}^q \eta_n^{l-q-1} \rho_0^{l-q-1} - d_{+mn}^q \sigma_n^{l-q-1} \rho_{20}^{l-q-1} \right) f_{1\theta} \rho_0 \frac{l-q}{f_1} \mathbf{e}_\theta p_{+mn} \Big] \Big|_{r\in\sigma_0} = 0. \qquad \text{(A.3)}
\end{aligned}$$

We assume that at the current step all coefficients of order $(l-1)$ and lower are known, so we isolate the

term of order l on the left-hand side, and move the remaining expression to the right-hand side, denoting it by the vector $\mathbf{S}_l$. We proceed analogously for the second boundary condition on the magnetic field and obtain Eqs. (10).

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