Expansion of the scattering phase function in Legendre polynomials

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Elements of the theory of angular momentum in the Rayleigh–Gans–Debye (RGD) approximation are used to derive an expansion of the phase function in Legendre polynomials for a single spherical particle and polydisperse spherical and randomly oriented spheroidal particles. The numerical calculations are then compared with rigorous results of the T-matrix method.

Introduction

Expansion of the elements of the scattering matrix into generalized spherical functions has been an efficient tool for solving single and multiple scattering problems.[1,2] If the expansion coefficients are known, then the elements of the scattering matrix can be estimated for a large set of scattering angles,[3] while the scattered fluxes are estimated for a large set of arbitrary solid angles[4] for different polarizations of the incident radiation with minimum computational expense.

Presently, the possibility of estimating these coefficients is limited to cases in which the rigorous theory can be applied, namely, nonspherical particles of even regular shapes.[5] This limitation bears on particle size and particle shape parameters.

The goal of the present paper is to fill this gap for optically "soft" particles whose properties satisfy the premises of the Rayleigh–Gans–Debye (RGD) theory,[6] and to derive the expansion coefficients of the scattering phase function for ensembles of spherical and randomly oriented spheroidal particles.

1. The Rayleigh–Gans–Debye approximation. Shape factor

Upon solution of the integral wave equation, the amplitude of the scattered wave in the far zone ($kR \gg 1$) can be represented as[7]

$$\mathbf{E}^{s}(\mathbf{r}) = -\frac{e^{ikR}}{kR}\,\mathbf{A}(\mathbf{n}_s, \mathbf{n}_i); \tag{1}$$

$$\mathbf{A}(\mathbf{n}_s, \mathbf{n}_i) = \frac{k^3}{4\pi}\int_V \{\mathbf{n}_s \times [\mathbf{n}_s \times \mathbf{E}(\mathbf{r}')]\} \times \times [(m_r^2(\mathbf{r}') - 1]\, e^{-ik\mathbf{n}_s\mathbf{r}'}\, dV, \tag{2}$$

where $k = 2\pi/\lambda$ is the wave number of the surrounding medium; m_r is the relative refractive index of the particle; λ is the wavelength of the incident radiation; R is distance to the observation point; $\mathbf{n}_i = (\theta_i, \varphi_i)$ and $\mathbf{n}_s = (\theta_s, \varphi_s)$ are direction (unit) vectors of propagation of the incident and scattered radiation, respectively; $\mathbf{E}(\mathbf{r}')$ is the time-independent electric field vector inside a particle, where the factor $e^{i\omega t}$ is suppressed for convenience. This expression is an exact integral expression for $\mathbf{E}^s(\mathbf{r})$ in terms of $\mathbf{E}(\mathbf{r}')$ inside a particle.

The form of the approximation of internal field of a particle is determined by approach taken. The Rayleigh–Gans–Debye theory is one such approximation, with the incident field used to approximate the internal one: $\mathbf{E}(\mathbf{r}') = \mathbf{e}_i\, e^{ik\mathbf{n}_i\mathbf{r}'}$ (here $\mathbf{e}_i$ is the unit polarization vector of the incident plane wave). In this case, equation (2) simplifies to

$$\mathbf{A}(\mathbf{n}_s, \mathbf{n}_i) = \frac{k^3}{4\pi}\{\mathbf{n}_s \times [\mathbf{n}_s \times \mathbf{e}_i]\} \times \times \int_V [m_r^2(\mathbf{r}') - 1]\, e^{-i\boldsymbol{k}_s\mathbf{r}'}\, dV, \tag{3}$$

where $\boldsymbol{k}_s = k(\mathbf{n}_i - \mathbf{n}_s)$.

The RGD approximation is applicable provided that[6]

$$|m_r - 1| \ll 1, \quad 2kr\,|m_r - 1| \ll 1, \tag{4}$$

where r is particle size.

To describe the electromagnetic wave scattered by a homogeneous spherical particle and propagating along the z axis, we use a right-handed coordinate system with origin inside a scatterer.

Formula (3) expresses in matrix form the amplitude scattering matrix[6]:

$$\begin{bmatrix} E_1^s \\ E_2^s \end{bmatrix} = -\frac{e^{ikR}}{kR}\begin{bmatrix} S_{11} & 0 \\ 0 & S_{22} \end{bmatrix}\begin{bmatrix} E_1^i \\ E_2^i \end{bmatrix}, \tag{5}$$

where $S_{11}(\theta_s) = (m_r^2 - 1)\, f(\theta_s)$; $S_{22}(\theta_s) = (m_r^2 - 1)\, f(\theta_s) \times \times \cos(\theta_s)$, θ_s is the scattering angle, E_1 and E_2 are the coordinates of the electric field vector in a basis with the basis vectors parallel and perpendicular to the scattering plane;

$$f(\theta_s) = \frac{k^3}{4\pi}\int_V e^{i\mathbf{k}_s\mathbf{r}}\, dV. \tag{6}$$

For homogeneous particles of some shapes, shape factors (6) are known, have an explicit form, and are given in Ref. 8.

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To solve the problem of concern here, we used an unconventional expression for the shape factor of a homogeneous spherical particle. Neglecting details of the derivation, based on the representation of a plane wave in terms of the Wigner function and use of the addition theorem,[9] upon integration of (6) we obtain the separable equation

$$f(\theta_s) = \sum_{n=0}^{\infty} R_n(kr)\, d^n_{00}\,(\theta_s), \quad (7)$$

$$R_n(kr) = \frac{k^3 r^3}{2}(2n+1)\{j_n^2(kr) - j_{n-1}(kr)\, j_{n+1}(kr)\}, \quad (8)$$

where $j_n(kr)$ are spherical Bessel functions. The Wigner functions and Legendre polynomials are related as

$$P_n\,(\cos\theta) = d^n_{00}\,(\theta).$$

2. The coefficients of expansion of the scattering phase function into Legendre polynomials

In the RGD approximation, the only independent element of the scattering matrix is the intensity of the scattered radiation in the case of unpolarized incident radiation of unit intensity, namely:

$$Z_{11}(\theta_s) = 1/2\ |m_r^2 - 1|^2\ |f(\theta_s)|^2\ [1 + \cos^2(\theta_s)], \quad (9)$$

and the corresponding scattering phase function is

$$F_{11}(\theta_s) = \frac{4\pi}{C_{scat}} Z_{11}(\theta_s), \quad (10)$$

where C_{scat} is the scattering coefficient (cross section).

Neglecting details of the derivation, the final expressions for the expansion coefficients are

$$Z_{11}(\theta_s) = \sum_{n=0}^{\infty} a_n\, P_n(\cos\theta_s), \quad (11)$$

$$a_n = \frac{4}{3}\alpha_n + \frac{2}{3}\sum_{n'=|n-2|}^{n+2}\left[C^{n'0}_{n020}\right]^2 \alpha_{n'}, \quad (12)$$

$$\alpha_m = |m_r^2 - 1|^2 \sum_{n=0}^{\infty}\ \sum_{n'=|n-m|}^{n+m} R_n(kr)\, R_{n'}(kr)\left[C^{m0}_{n0n'0}\right]^2,$$

$$m = 0,\ 1,\ 2,\ \ldots\ . \quad (13)$$

Two useful properties of the expansion coefficients are[1]

$$a_0 = \frac{C_{scat}}{4\pi}, \quad \frac{a_1}{3} = \langle\cos\theta_s\rangle. \quad (14)$$

Normalization of the coefficients a_n by a_0 gives the expansion coefficients of the scattering phase function (10).

3. Polydisperse spherical and randomly oriented spheroidal particles

Formulas of expansion coefficients for polydisperse spherical particles are analogous to (12) and (13) except for the requirement of averaging $R_n(kr)R_n(kr)$ over particle ensemble.

In the RGD approximation, the randomly oriented prolate and oblate spheroidal particles can be made optically equivalent to polydisperse spherical particles using an appropriate weighting function[10]:

$$\rho(a, b, r) = \begin{cases} \dfrac{a^4 b}{e}\dfrac{1}{r^5\sqrt{r^2 - a^2}}, & a \le r \le b, \\[2ex] \dfrac{a^3 b^2}{e}\dfrac{1}{r^5\sqrt{a^2 - r^2}}, & b \le r \le a, \end{cases} \quad (15)$$

where b and a are the vertical and horizontal semi-diameters; $e = \sqrt{\varepsilon^2 - 1/\varepsilon}$, where ε is the shape parameter which is defined as the ratio of the larger to the smaller semi-diameter. Thus, the problem of finding the expansion coefficients for randomly oriented spheroids essentially reduces to that of determining the expansion coefficients for polydisperse spherical particles. In the case of polydisperse, randomly oriented spheroids with size distribution $f(a, b)$, the weighting function of the equivalent ensemble of spherical particles has the form of a convolution[11]: $f(a, b)*\rho(a, b, r)$.

4. Calculation results

The utility of the results obtained in region (4) can be tested by comparing them with calculations based on the T-matrix method.[12] Figure 1 presents calculations of the scattering phase function for randomly oriented spheroids. The shape effect for equivalent-volume ($kr = 10$) particles is shown in Fig. 2.

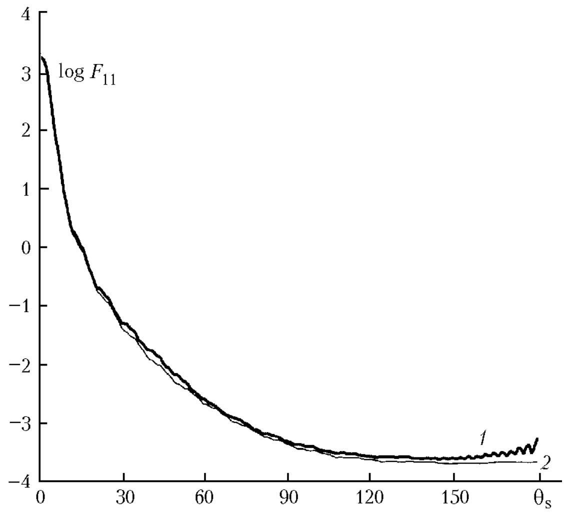

Fig. 1. Scattering phase functions of randomly oriented monodisperse oblate spheroids obtained using the T-matrix method (curve *1*) and the RGD approximation (curve *2*): $ka = 60$, $a/b = 3$, $m_r = 1.01$.

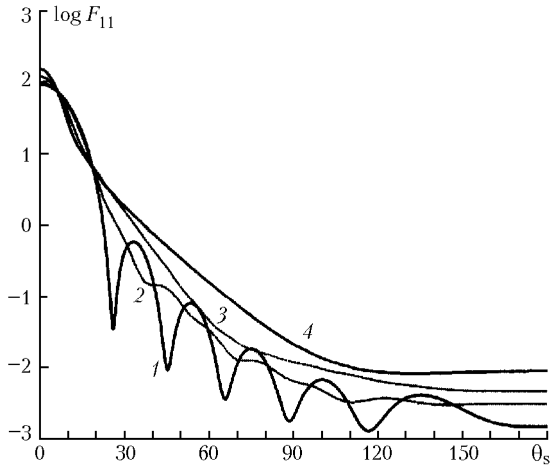

Fig. 2. Scattering phase function of monodisperse randomly oriented equivalent-volume (kr = 10) oblate spheroids with ε = 1.1 (curve *1*), ε = 2 (curve *2*), ε = 5 (curve *3*), and ε = 10 (curve *4*).

Thus, in the applicability region of RGD theory the obtained results can be used to estimate the expansion coefficients of the scattering phase function for the above-mentioned particle ensembles without limitations on particle size or particle shape parameters.

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