S-approximation for the small-angle scattering phase function

A.Ya. Perelman and I.G. Moseev

St. Petersburg State Forestry Engineering Academy

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Within the framework of the soft particle approximation (SA), the small scattering angle representation for the Mie amplitude functions is constructed. The general analytical criterion of transition from SA of any optical characteristic to its anomalous diffraction approximation (ADA) is formulated. The ADA for the small-angle scattering phase function is determined and its applicability domain is investigated. The ADA and the Kirchoff approximation are shown to have the same asymptotic behavior.

Investigation of scattering and extinction properties of spherical particles is needed in solving radiative transfer and remote sensing problems, as well as to study optical and microphysical properties of aerosol and hydrosol. Calculations by the Mie theory present no principal difficulties now, but to understand the physics of the phenomenon, it is reasonable to consider approximate equations that are valid in some limiting cases.¹ Such equations based on the physical meaning of their domain of applicability correspond, for example, to the anomalous diffraction approximation (ADA) proposed by van de Hulst,² Rayleigh–Gans approximation (RGA), Kirchoff approximation (KA),^{1–3} KA with correction factor.^{3,4}

The method for approximate summation of the Mie series for soft particles (S-approximation, SA) was considered in Refs. 5 and 6. This method is based on formal substitution of the scattering coefficients by their average values (the error of averaging uniformly tends to zero as the complex refractive index m tends to unity) and the following exact summation of the transformed Mie series with the use of addition theorems for spherical Bessel functions. In Refs. 7 and 8 it was shown that SA gives a small error in the range of the size parameter values x and the values of the refractive index m, that allow the optical properties of actual disperse media to be investigated.

The SA turned out to be useful in solving some problems of light scattering.⁹ In particular, the SA was used in studying the scattering phase function of infinite dielectric cylinders,¹⁰ in the theory of scalar diffraction,¹¹ in the study of energy characteristics of scattering,¹² in establishment of relations between various optical approximations.¹³

Let us denote

$$\rho = 2(y-x); R = 2(y+x); y = mx,$$
 (1)

 $a_{kn}(m,x)$ are the scattering coefficients; θ is the scattering angle; $\mu = \cos\theta$; $A_k(m, x, \mu)$ are the amplitude functions, $\overline{n} = n(n+1)$, $\dot{n} = n+0.5$ (k = 1, 2; n = 1, 2, ...). In some cases independent variables are not explained.

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Accurate to θ^4 , the small-angle amplitude functions have the form⁸:

$$A_{1}(m, x, \mu) = \sigma - 0.25(1 - \mu)(3\sigma_{1} + \sigma_{2} - 2\sigma),$$

$$A_{2}(m, x, \mu) = \sigma - 0.25(1 - \mu)(\sigma_{1} + 3\sigma_{2} - 2\sigma),$$
(2)

where

$$\sigma = \sum \dot{n}(a_{1n} + a_{2n}), \quad \sigma_k = \sum \overline{n} \dot{n} a_{kn}. \tag{3}$$

Now, find SA of the functions (2). Using the results of Refs. 6 and 8, we obtain

$$\sigma_1 = x^{-2} (H_{11} - iH_{13}), \quad \sigma_2 = x^{-2} (H_{22} - iH_{24}). \tag{4}$$

Here

$$H_{11} = x^{2}\alpha(y,x) + y^{2}\alpha(x,y) - 2xy\beta(x,y),$$

$$H_{22} = y^{2}\alpha(y,x) + x^{2}\alpha(x,y) - 2xy\beta(x,y),$$

$$H_{13} = x^{2}\delta(x,y) + y^{2}\gamma(x,y) - xy\varepsilon(x,y),$$

$$H_{24} = y^{2}\delta(x,y) + x^{2}\gamma(x,y) - xy\varepsilon(x,y),$$
(5)

where

$$\alpha(x,y) = \sum \overline{n} \dot{n} \dot{\psi}_{n}'^{2}(x) \psi_{n}^{2}(y);$$

$$\beta(x,y) = \sum \overline{n} \dot{n} \dot{\psi}_{n}'(x) \psi_{n}(x) \psi_{n}'(y) \psi_{n}(y);$$

$$\gamma(x,y) = \sum \overline{n} \dot{n} \dot{\psi}_{n}'(x) \chi_{n}'(x) \psi_{n}^{2}(y);$$

$$\delta(x,y) = \sum \overline{n} \dot{n} \dot{\psi}_{n}'(x) \chi_{n}(x) \psi_{n}'^{2}(y);$$

$$\epsilon(x,y) = \sum \overline{n} \dot{n} [\psi_{n}'(x) \chi_{n}(x) + \psi_{n}(x) \chi_{n}'(x)] \psi_{n}'(y) \psi_{n}'(y).$$
(6)

The exact sums of the series (6) can be presented as

$$\sum_{l} \left[f_{l}(m,\rho) - (-1)^{l} f_{l}(-m,R) \right] x^{l}, \tag{7}$$

where f_l are expressed in terms of the functions

$$t_{1}(x) = x^{-1}\sin x, \qquad d_{1}(x) = x^{-1}\cos x,$$

$$t_{2}(x) = x^{-2}(1-\cos x), \qquad d_{2}(x) - x^{-2}\sin x,$$

$$t_{3}(x) = x^{-3}(\sin x - x\cos x), \quad t_{4}(x) = x^{-4}[x\sin x - 2(1-\cos x)],$$

$$cix = \int_{0}^{x} t^{-1}(1-\cos t)dt, \qquad six = \int_{0}^{x} t^{-1}\sin tdt. \qquad (8)$$

In its turn, the SA for the series σ is presented by Eq. (P5) (Refs. 7 and 8).

The ADA and RGA are particular cases of SA. $^{6-8}$ The following formal criteria of transition from SA to ADA and RGA are valid:

1. SA transforms into ADA if

$$\rho = 2(y - x)$$
 in $f_l(m, \rho)$

only as an argument of the functions (8),

$$y = x$$
 in other cases. (9)

2. SA transforms into RGA if

$$R = 2(y + x)$$
 in $f_l(-m, R)$

only as an argument of the functions (8),

$$y = x$$
 in other cases. (10)

Consider small-angle amplitude functions and the scattering phase function in ADA. In view of Eqs. (5), (6), and (9), we obtain

$$\sigma_1 = \sigma_2 = 2(\alpha - \beta) - (2\gamma - \varepsilon)i.$$
(11)

It follows herefrom that $A_k(m, x, \mu) = A(m, x, \mu)$, that is, unlike the SA, ADA does not allow the study of polarization effects. Using Eqs. (21), (11), (P4), and (P5), we obtain (x > 5)

$$A(m, x, \mu) = x^{2}(\tau + \delta i) - 0.25(1 - \mu) x^{4}(\gamma \tau + \delta i) .$$
(12)

Here

$$\tau = 0.5 + t_2 - t_1; \, \delta = d_2 - d_1; \, \gamma = \frac{1 + t_2}{2\tau}, \tag{13}$$

where $t_k = t_k(\rho)$ and $d_k = d_k(\rho)$ [see Eq. (8)]. The condition x > 5 is connected with the fact that an additional term depending on the functions (8) at $x = \rho$ should be taken into account in Eq. (12) at small size parameters x. Thus, accurate to $O(\theta^4)$ we have (x > 5)

$$|A(m, x, \mu)|^{2} = |A(m, x, 1)|^{2} q(m, x, \mu),$$

$$|A(m, x, 1)|^{2} = x^{4} (|\tau|^{2} + |\delta^{2}|),$$

$$q(m, x, \mu) = 1 - 0.5(1 - \mu)x^{2} \times$$

$$\times \frac{\gamma_{1}|\tau|^{2} + |\delta|^{2} + (\gamma_{1} + 1)(-\tau_{1}\delta_{2} + \tau_{2}\delta_{1}) + \gamma_{2}(\tau_{1}\delta_{1} + \tau_{2}\delta_{2})}{|\tau|^{2} + |\delta|^{2}},$$
(14)

where τ_1 , δ_1 , γ_1 and τ_2 , δ_2 , γ_2 are, respectively, real and imaginary parts of τ , δ , and γ determined in Eq. (13). The functions $|A(m, x, 1)|^2$ and $q(m, x, \mu)$ determine the radial and angular factors of the small-angle scattering phase function. Note that for dielectric spheres Eq. (14) gives

$$|A(m,x,\mu)|^{2} = x^{4} (\tau^{2} + \delta^{2}) - 0.5(1-\mu)x^{6} (\gamma\tau^{2} + \delta^{2}).$$
(15)

In this equation, designations from Eq. (13) are used and it is taken into accounts that τ , δ , and γ are real at m = Re m.

Consider the particular case (15) corresponding to large phase shifts ρ . Under this condition, we can assume $\tau = 0.5$, $\delta = 0$, and $\gamma = 1$. We have

$$\left|A^{\infty}(x,\mu)\right|^{2} = 0.25x^{4}[1-x^{2}\sin^{2}(0.5\theta)], \qquad (16)$$

where the designation

$$\left|A^{\infty}(x,\mu)\right| = \lim_{\rho \to \infty} \left|A(m,x,\mu)\right|, \qquad (17)$$

accounting for the independence of the considered limit on the refractive index *m* is taken into consideration. In its turn, the KA for amplitude functions (2) can be written as²:

$$A^{\mathrm{Kir}}(x,\mu) = x \sin^{-1} \theta J_1(x \sin \theta) . \tag{18}$$

In view of Eqs. (16) and (18), ADA and KA coincide at small scattering angles accurate to $O(\theta^4)$, since under this assumption Eq. (18) gives

$$\left|A^{\rm Kir}(x,\mu)\right|^2 = 0.25x^4 \left(1 - 0.25x^2 \sin^2 \theta\right).$$
 (19)

It should be noted that ADA, unlike KA, takes into account the dependence of the amplitude Mie functions on the refractive index m.

The scattering phase function of a spherical particle can be presented in the form

$$\begin{cases}
I(m, x, \mu) = i(m, x) Q(m, x, \mu), \\
i(m, x) = i_1(m, x, 1) + i_2(m, x, 1), \\
Q(m, x, \mu) = \frac{i_1(m, x, \mu) + i_2(m, x, \mu)}{i(m, x)},
\end{cases}$$
(20)

where the functions $i_k(m, x, 1)$ are equal to the squared absolute values of the amplitude Mie functions.² In view of Eqs. (14) and (20) and the equality $i_k(m, x, 1) =$ = i(m, x, 1), the errors in the radial and angular factors for ADA are given by the following equations:

$$E(m, x) = 1 - \frac{|A(m, x, 1)|^2}{i(m, x, 1)}$$
(21)

and

$$e(m, x, \mu) = 1 - \frac{q(m, x, \mu)}{Q(m, x, \mu)}.$$
 (22)

The error of the radial factor (21) was estimated in Ref. 2. It is essential that this error becomes negligibly small for any values of the size parameter x and the refractive index m = n - ik in any case in the range $n \le 2$ and $k \le 0.5$ if we use the representation of the radial factor $|A(m, x, 1)|^2$ derived in Refs. 14 and 15.

Let the designation $\theta_{\max} = \theta_{\max}(m, x)$ to stand for the exact upper boundary of the scattering angles determined by the inequality

$$|e(m, x, \mu)| \le 0.1$$
. (23)

The function θ_{\max} weakly depends on the real part n of the refractive index and is almost insensitive to small variations of its imaginary part k. Inside the admissible range $0 \le \theta \le \theta_{\max}$, the error of the angular factor varies rather slowly, but in the range $\theta > \theta_{\max}$ it increases quickly. The behavior of the function θ_{\max} is illustrated in Fig. 1. Figure 2 shows the typical angular Mie factors.



The procedure of transition from SA to ADA is determined by Eq. (9). If the condition (9) is fulfilled, the results obtained in SA simplify significantly. ADA representations of optical characteristics do not include functions depending on R; besides, ADA does not include integral sine and cosine. The transition from SA to ADA yields new representations (14) and (15) for the amplitude functions. The well known van de Hulst equation for the extinction efficiency factor²

$$Q_{\text{ext}} = 4 \operatorname{Re} K(i\rho), \ K(w) = 0.5 + w^{-1}e^{-w} + w^{-2}(e^{-w} - 1)$$
(24)

follows from Eqs. (12) and (13) and the optical theorem, since

$$x^{-2}\operatorname{Re} A(m, x, 1) = \operatorname{Re}(\tau + \delta i).$$
(25)

On the other hand, ADA is insensitive to the degree of polarization, and one should use SA to study the scattering phase matrix. It should be noted that the use of the transition equation (10) allows the RGA for $Q_{\rm ext}$ to be refined in the case of absorbing particles.

SA keeps the analytical structure of the exact solution, as well as its shortwave and longwave asymptotics,^{7,8,14,15} and therefore it allows description of the basic properties of light scattering by spherical particles.

APPENDIX

Series used in ADA

Applying Eqs. (8) and (9) and using the addition theorem and differential equation for the spherical Bessel functions, we obtain

$$\begin{aligned} \alpha &= \frac{1}{64} [4x^4 - 11x^2 + (6x^2 - 0.5)c^- + 12x^2T_1 + \\ &+ (24x^4 - 4x^2)T_2 - 40x^4(T_3 + T_4) + 6x^2t_1 + \\ &+ (8x^4 - 6x^2)t_2 - 24x^4(t_3 + t_4)], \\ \beta &= \frac{1}{64} [-6x^2 + (6x^2 - 0.5)c^- + 14x^2T_1 + \\ &+ (40x^4 - 6x^2)T_2 - 56x^4(T_3 + T_4) - 6x^2t_1 + \\ &+ (-8x^4 + 6x^2)t_2 + 24x^4(t_3 + t_4)], \end{aligned}$$
(P1)
$$\gamma &= \delta = \frac{1}{64} [(6x^2 - 0.5)s^+ + 7x^2D_1 + \\ &+ (-16x^4 + x^2)D_2 + (8x^4 + 6x^2)d_1 + \\ &+ (-8x^4 - 6x^2)d_2 + 8x^3t_3], \end{aligned}$$
$$z &= \frac{1}{32} [(6x^2 - 0.5)s^+ + 7x^2D_1 + (-16x^4 + x^2)D_2 + \\ &+ 10x^2d_1 - 10x^2d_2 + 8x^3t_3], \end{aligned}$$

where

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$$t_k(\rho) = t_k; \ d_k(\rho) = d_k; \ t_k(R) = T_k; \ d_k(R) = D_k;$$

$$c^- = ciR - ci\rho; \qquad s^+ = siR + si\rho.$$
(P2)

Taking into account Eq. (P1) and the identity

$$16x^4(T_3 + T_4) = 2x^2T_1 + (16x^4 - 2x^2)T_2 - x^2$$
 (P3)

we obtain

$$\alpha - \beta = \frac{1}{32} [2x^2 - 3 + 6t_1 + (8x^2 - 6)t_2 - 24x^2(t_3 + t_4)]x^2;$$

$$2\gamma - \delta = \frac{1}{8} (2x^4 - x^2)(d_1 - d_2).$$
 (P4)

Similarly, we can obtain

$$\sigma = x^2 [0.5 - t_1 + t_2 - (d_1 - d_2)i].$$
 (P5)

A.Ya. Perelman and I.G. Moseev

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