Improved S-approximation for dielectric particles ⋆

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Abstract

The range of the applicability of the soft particles approximation (S-approximation) has been extended by means of the procedure which may be considered as a specific form of the analytic continuation. The initial element is represented by the standard version of the approximation while the branch of the continuation should be chosen in correspondence with the short wavelength asymptotic of the optical characteristic under consideration. As for the extinction efficiency of dielectric spherical particles, the improved version of the S-approximation fairly well describes the behaviour of Mie curves for particles with the refractive indices up to 2.0 or more and may be useful in order to get in the analytical form the "smoothed" Mie curves when the ripple-type fluctuations were averaged.

The leading role of the van de Hulst approximation both for the electric and magnetic components of the extinction efficiency has been shown.

Key words: Light scattering; Extinction efficiency; van de Hulst approximation

1 Introduction

The theory of anomalous diffraction was worked out by van de Hulst in [1] and [2]. Within the framework of this theory, by the subtle physical reasoning based on the Huygens' principle, the very effective representations for the

⋆ To the memory of Hendrik Christoffel van de Hulst.

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efficiency factors and amplitude functions have been derived (see [1], [3]). The final expressions of the van de Hulst approximation (vdHA) describe the main features of the scattering phenomenon. On the view of their elegance and simplicity the vdHA presents a proper tool when investigating the problem of light scattering by spherical particles exposed to a plane wave (the Mie theory).

In this paper, we discuss the method to transform and sum the series which represent the optical characteristics in the Mie problem. As a result, we are able to give the mathematical substantiation of the theory of anomalous diffraction and formulate the conditions of its applicability without using any physical hypotheses. New approximation represents the results of Mie theory to a fairly high degree of accuracy within the wide range of the input parameters. The principal part of the presented approximation for the extinction efficiency factor coincides with that of the vdHA.

Let us introduce the basic notations: $x = 2\pi a/\lambda$ is the size parameter (a the radius of a sphere, λ the wavelength of the incident radiation), m is the relative refractive index,

$$\rho = 2(m-1)x, \qquad R = 2(m+1)x, \qquad s_\tau = \frac{\sin\tau}{\tau},$$

$$c_\tau = \frac{1-\cos\tau}{\tau^2}, \qquad \mathrm{ci}(\tau) = \int\limits_0^\tau \frac{1-\cos t}{t}\mathrm{d}t, \qquad c^\tau = \frac{\mathrm{ci}(\tau)}{\tau^2}\,.$$

Here, ρ and R is a phase shift of the central ray for transmitted and backscattered radiation.

The most useful result obtained in the theory of anomalous diffraction (see [3]) is the well-known expression for extinction efficiency factor of non-absorbing spheres, namely,

$$Q_{\mathrm{ext}}^{\mathrm{vdHA}}(m,x) = 2 - 4s_\rho + 4c_\rho\,. \tag{1}$$

2 Description of methods

2.1 General definitions

The scattering characteristics in the Mie theory are expressed in terms of series depending on the electric a_{1n} and magnetic a_{2n} coefficients. For example, the efficiency factor for extinction is given by series [3]

$$Q_{\text{ext}} = \frac{2}{x^2}\mathrm{Re}\sum_{n=1}^{\infty}(2n+1)(a_{1n}+a_{2n})\,. \qquad (2)$$

The Mie coefficients can be written in the form

$$a_{1n} = \frac{h_{1n}^2 - ih_{1n}h_{3n}}{h_{1n}^2 + h_{3n}^2}\,, \qquad a_{2n} = \frac{h_{2n}^2 - ih_{2n}h_{4n}}{h_{2n}^2 + h_{4n}^2}\,, \qquad (3)$$

where

$$\begin{cases} h_{1n} = x\psi_n'(mx)\psi_n(x) - mx\psi_n(mx)\psi_n'(x)\,, \\ h_{2n} = mx\psi_n'(mx)\psi_n(x) - x\psi_n(mx)\psi_n'(x)\,, \\ h_{3n} = x\psi_n'(mx)\chi_n(x) - mx\psi_n(mx)\chi_n'(x)\,, \\ h_{4n} = mx\psi_n'(mx)\chi_n(x) - x\psi_n(mx)\chi_n'(x) \end{cases} \qquad (4)$$

and $\psi_n(z), \chi_n(z), \psi_n'(z), \chi_n'(z)$ are the Riccati-Bessel functions and their first derivatives.

By definition, the soft particles approximation (the S-approximation, SA) is based on the assumption that the denominators in Eq. (3) can be replaced by the following expressions

$$h_{1n}^2 + h_{3n}^2 \approx \frac{|m|x^2}{g(|m|,x)}\,, \qquad h_{2n}^2 + h_{4n}^2 \approx \frac{|m|x^2}{g(|m|,x)}\,, \qquad (5)$$

where

$$g(|m|,x) = \mathcal{O}(1) \qquad \text{as} \qquad x \longrightarrow \infty\,. \qquad (6)$$

The above suppositions reflect the behaviour of Wronskian for the Riccati-Bessel functions and are justified by their asymptotic behaviour. In the long run, the specific choice of the smoothing function $g(|m|,x)$ should be determined by the short wavelength approximation of the optical characteristic under consideration.

Some series that occur in the scattering theory can be summed in the SA. Here, we shall confine ourselves to the case of non-absorbing particles [$m = \mathrm{Re}(m)$].

The optical characteristics in the SA are represented as the linear combination of functions $\beta(l)B(\tau)$, where $B(\tau)$ are the basic functions of one variable τ

and the coefficients $\beta(l)$ are the weight functions. The products $\beta(l)B(\tau)$ are computed at $\tau=\rho$, $l=m$ and $\tau=R$, $l=-m$. The function $B(\tau)$ is called the basic one if

$$B(\tau)=\mathcal{O}(\tau^k)\,,\qquad k\geq 0\qquad (\tau\longrightarrow 0)$$

and $B(-\tau)=B(\tau)$ in the case of non-absorbing particles. Every weight function $\beta(l)$ is the linear combination of l^k (k are integers) with the constant coefficients satisfying the condition $\beta(-1)=0$. The SA is named of the standard form if

$$\beta(1)\neq 0$$

for all the weight functions. This form of the SA is often convenient to analyse the results obtained.

As a preliminary, we put

$$g(m,x)=1\,. \tag{7}$$

From Eqs. (3), (5) and (7) it follows that

$$a_{1n}=\frac{h_{1n}^2}{mx^2}\,,\qquad a_{2n}=\frac{h_{2n}^2}{mx^2} \tag{8}$$

in the considered version of the SA.

2.2 S-approximation in the standard form

Using the assumption given by Eq. (8) we can sum the series for electric and magnetic components

$$\sigma_1=\sum_{n=0}^{\infty}(n+0.5)a_{1n}\,,\qquad \sigma_2=\sum_{n=0}^{\infty}(n+0.5)a_{2n}\,. \tag{9}$$

After some reductions based on the addition theorem for the Bessel functions (see [4]) it is possible to find

$$\begin{cases}\sigma_1=\dfrac{x^2}{32m^2}\left\{b(m)\left[b_0^2(m)\mathcal{H}(\rho)+\dfrac{2b_0(m)\mathcal{H}_1(\rho)}{x^2}+\dfrac{\mathcal{H}_2(\rho)}{8x^4}\right]-\right.\\ \qquad\left. b(-m)\left[b_0^2(m)\mathcal{H}(R)+\dfrac{2b_0(m)\mathcal{H}_1(R)}{x^2}+\dfrac{\mathcal{H}_2(R)}{8x^4}\right]\right\}\,,\\ \sigma_2=\frac{x^2}{8}\left[b(m)\mathcal{H}(\rho)-b(-m)\mathcal{H}(R)\right]\,,\end{cases} \tag{10}$$

where

$$
\begin{cases}
\mathcal{H}(\tau) = 2 - 4s_\tau + 4c_\tau \, , \\
\mathcal{H}_1(\tau) = \tau^2[2s_\tau + 2c_\tau + \mathrm{ci}(\tau)] \, , \\
\mathcal{H}_2(\tau) = -\tau^4(1 + 2s_\tau + 6c_\tau + 8c^\tau)
\end{cases}
\tag{11}
$$

and

$$
b(m) = \frac{(m+1)^2}{4} \, , \qquad b_0(m) = m^2 + 1 \, . \tag{12}
$$

Using the expressions

$$
h_{j\,0}^2 = \frac{x^4(m^2-1)^2}{2}\left[c_\rho + c_{\mathrm{R}} + (-1)^{j-1} s_{\rho/2} s_{\mathrm{R}/2}\right] \, , \qquad j = 1, 2 \, , \tag{13}
$$

Eqs. (2) and (8) – (10), the standard form of the SA for the extinction efficiency factors can be derived

$$
\begin{aligned}
Q_{\mathrm{ext}}^{\mathrm{SA}}(m, x) &= \beta(m)\mathcal{H}(\rho) + \frac{\beta_1(m)\mathcal{H}_1(\rho)}{x^2} + \frac{\beta_2(m)\mathcal{H}_2(\rho)}{x^4} \\
&- \left(\beta(-m)\mathcal{H}(R) + \frac{\beta_1(-m)\mathcal{H}_1(R)}{x^2} + \frac{\beta_2(-m)\mathcal{H}_2(R)}{x^4}\right) \\
&\quad + \beta_3(m)\mathcal{H}_3(\rho) + \beta_3(-m)\mathcal{H}_3(R) \, .
\end{aligned}
\tag{14}
$$

Here, $\mathcal{H}(\tau)$, $\mathcal{H}_1(\tau)$ $\mathcal{H}_2(\tau)$ and $\mathcal{H}_3(\tau) = \tau^2 c_\tau$ are the basic (van de Hulst) functions, and

$$
\begin{cases}
\beta(l) = \dfrac{(l^4 + 6l^2 + 1)b(l)}{8l^2} \, , & \beta_1(l) = \dfrac{(l^2+1)b(l)}{4l^2} \, , \\[2ex]
\beta_2(l) = \dfrac{b(l)}{64l^2} \, , & \beta_3(l) = -\dfrac{b(l)}{l}
\end{cases}
\tag{15}
$$

are the weight functions. Substituting Eq. (15) into Eq. (14) we have

$$
\begin{aligned}
Q_{\mathrm{ext}}^{\mathrm{SA}}(m, x) &= \frac{1}{8m^2} \\
&\times \left\{ b(m)\left[\left(m^4 + 6m^2 + 1\right)\mathcal{H}(\rho) + \frac{2b_0(m)\mathcal{H}_1(\rho)}{x^2} + \frac{\mathcal{H}_2(\rho)}{8x^4}\right] \right. \\
&\left. -b(-m)\left[\left(m^4 + 6m^2 + 1\right)\mathcal{H}(R) + \frac{2b_0(-m)\mathcal{H}_1(R)}{x^2} + \frac{\mathcal{H}_2(R)}{8x^4}\right]\right\}
\end{aligned}
\tag{16}
$$

$$-\frac{1}{m}[b(m)\mathcal{H}_3(\rho)+b(-m)\mathcal{H}_3(R)]\,.$$

With the aid of the relation (see [5])

$$\mathrm{ci}(\tau)=\gamma+\ln\tau-\frac{\sin\tau}{\tau}+\frac{\cos\tau}{\tau^2},\quad(\tau\gg 1),\tag{17}$$

where γ is the Euler constant, and Eqs. (9) – (13) we can find the limits characterizing the short wavelength approximations of the electric and magnetic components in the SA

$$\begin{cases}\lim\limits_{x\to\infty}\left[\dfrac{2}{x^2}\mathrm{Re}\sum\limits_{n=1}^{\infty}(2n+1)a_{1n}\right]=\dfrac{1}{4}\left[\dfrac{b_0^2(m)+(m^2-1)^2}{m}+\right.\\ \qquad\qquad\qquad\qquad\left.\dfrac{b_0(m)(m^2-1)^2}{m^2}\ln\left|\dfrac{m-1}{m+1}\right|\right], \\ \lim\limits_{x\to\infty}\left[\dfrac{2}{x^2}\mathrm{Re}\sum\limits_{n=1}^{\infty}(2n+1)a_{2n}\right]=m\,.\end{cases}\tag{18}$$

By virtue of Eqs. (2) and (18) we have

$$\mathcal{S}(m)=\lim_{x\to\infty}Q_{\rm ext}^{\rm SA}(m,x)=\frac{b_0^2(m)}{2m}+\frac{b_0(m)(m^2-1)^2}{4m^2}\ln\left|\frac{m-1}{m+1}\right|.\tag{19}$$

2.3 S- and van de Hulst approximations

The SA can be used in order to derive the various approximations known in the light scattering theory. As for the vdHA, it is convenient to use the SA in its standard form. Let us illustrate this fact in the case of the extinction efficiency factor.

The vdHA is known to be valid if

$$m-1\ll 1\,,\tag{20}$$

$$x\gg 1\,,\tag{21}$$

while the phase shift $\rho=2(m-1)x$ being arbitrarily fixed (see [3]). The condition of Eq. (20) for the SA is realized by substitution of $m=1$ into the weight functions given by Eq. (14). On the basis of Eqs. (12) and (15) we obtain

$$Q_{\rm ext}^{\rm SA}=\mathcal{H}(\rho)+\frac{\mathcal{H}_1(\rho)}{2x^2}+\frac{\mathcal{H}_2(\rho)}{64x^4}\,.\tag{22}$$

Then, the condition of Eq. (21) for the SA is realized by retaining in Eq. (22) its principal term as x tends to the infinity. Hence, we have $Q_{\rm ext}^{\rm SA} = \mathcal{H}(\rho)$, where ρ adopts the arbitrary value.

2.4 Non-standard form of the S-approximation

In [6] the extinction efficiency factor for dielectric particles has been derived in the following form

$$Q_{\rm ext}^{\rm SA}(m,x) = \frac{1}{2m}\left[(m^2+1)^2 + \frac{\omega(m,\rho)-\omega(-m,R)}{2m}\right], \tag{23}$$

where

$$\omega(m,\tau) = a(m){\rm ci}(\tau) + a_0(m)c^\tau + a_1(m)s_\tau + a_2(m)c_\tau \tag{24}$$

and

$$\begin{cases} a(m) = (m^2-1)^2(m^2+1)\,, \\ a_0(m) = -2(m^2-1)^2(m-1)^2\,, \\ a_1(m) = (m+1)^2(m^4-2m^3-2m^2-2m+1)\,, \\ a_2(m) = -a_0(m) - a_1(m)\,. \end{cases} \tag{25}$$

This non-standard [since $a(1) = a_0(1) = 0$] form of the SA written in terms of the basic functions $\tau^0 = 1$, ${\rm ci}(\tau)$, c^τ, s_τ and c_τ is suitable to show that the SA for the extinction efficiency factors turns into the Rayleigh-Gans approximation if

$$m - 1 \ll 1 \qquad \text{and} \qquad \rho \ll 1\,. \tag{26}$$

To prove this fact, we have to keep the basic functions up to $B(\rho) = \mathcal{O}(\rho^k)$ and the weight functions up to $\beta(m) = \mathcal{O}((m-1)^k)$ with $k \leq 2$ as ρ and $m-1$ become zero. But the main thing is that the SA in the form given by Eqs. (23) – (25) presents the conventual tool for the numerical calculations. It will be also used in the new version of the SA discussed below.

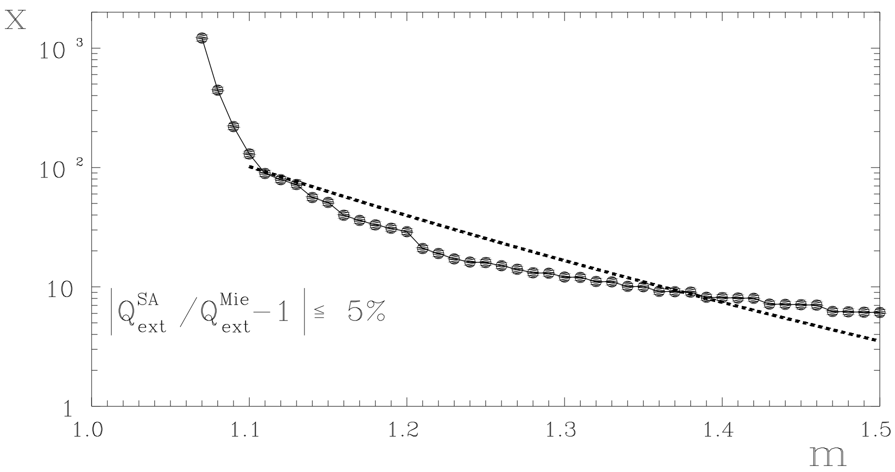

Fig. 1. Values of parameter x at which the efficiency factors in the S-approximation [Eqs. (23) – (25)] are calculated with an accuracy of 5 %. The dashed curve shows the power law approximation described by Eq. (27).

2.5 Improved form of the S-approximation (ISA)

The extinction factors calculated using the Mie theory and the S-approximation [Eqs. (23) – (25)] are compared in Fig. 1. It shows the range of the size parameter x in which both methods yield the results coinciding within 5 %. If $1.1 \leq m \leq 1.5$ this condition is satisfied if

$$0 \leq x < x(m)\,, \qquad x(m) \approx 290\, m^{-11}\,. \tag{27}$$

To improve the SA it needs to consider more carefully the short wavelength asymptotic of the amplitude functions. In the correspondence with Eq. (19) we replace Eq. (8) by the following one

$$a_{1n} = \frac{h_{1n}^2}{mx^2}\, g(m,x)\,, \qquad a_{2n} = \frac{h_{2n}^2}{mx^2}\, g(m,x)\,, \tag{28}$$

where

$$g(m,x) = 1 - f(m,x) + \frac{2}{\mathcal{S}(m)} f(m,x)\,, \tag{29}$$

$$f(m,x) = \exp\left[-\frac{0.01\,\exp(4m)\,x(m)}{x}\right]. \tag{30}$$

Thus, the improved form of the S-approximation for the extinction efficiency factors can be written as

$$Q_{\rm ext}^{\rm ISA}(m, ux(m)) = \left[1 - \frac{\mathcal{S}(m) - 2}{\mathcal{S}(m)} \exp\left(-\frac{0.01\exp(4m)}{u}\right)\right] Q_{\rm ext}^{\rm SA}(m, ux(m)). \quad (31)$$

Here, $u = x/x(m)$ is the size parameter in the scale of $x(m)$, the expressions for $Q_{\rm ext}^{\rm SA}(m, x)$ and $\mathcal{S}(m)$ are given by Eqs. (23) – (25) and Eq. (19), respectively.

3 Numerical results and discussion

We calculated the extinction efficiency factors $Q_{\rm ext}$ using the Mie theory and different approximations for the several refractive indices in the range from $m = 1.1$ to $m = 2.0$. Such refractive indices cover the interval of m typical for biological particles, sea water suspensions, water and water ice in the visible region and various silicates. The results are shown in Figs. 2 and 3.

As follows from Fig. 2, both the ISA and the vdHA deviate significantly from Mie curves for very small size parameters x and $m > 1.5$. In this case the condition given by Eq. (21) is not satisfied and the Rayleigh approximation must be used. For larger size parameters (and phase shifts) the ISA and the vdHA begin to work being the difference between the exact theory and approximations reduces with the growth of ρ (see Fig. 3). Note that in all cases the extinction produced by the vdHA is smaller than that of the Mie theory while the ISA reproduces very well both the position and the height of maxima and minima on the extinction curve. The latter is explained by the correction described by Eqs. (29) – (31).

However, the S-approximation cannot reproduce the small-scale ripple structure superimposed on the major oscillations as seen on the Mie extinction curves. These ripple-like fluctuations result from the resonances of virtual modes and are much better seen for the dielectric particles with large refractive indices (Figs. 2 and 3). The SA is based on the assumption that the denominators of the Mie coefficients are replaced by some expressions independent of the subscript n [see Eqs. (3) and (5)]. Therefore, it cannot reproduce the ripple structure but may be considered as the method of the construction of the *smoothed* Mie curves.

Figure 4 illustrates the relative accuracy of the van de Hulst and improved S-approximations given by the equation

$$\varepsilon = \frac{Q_{\rm ext}^{\rm Mie}}{Q_{\rm ext}^{\rm vdHA,\,ISA}} - 1\,. \quad (32)$$

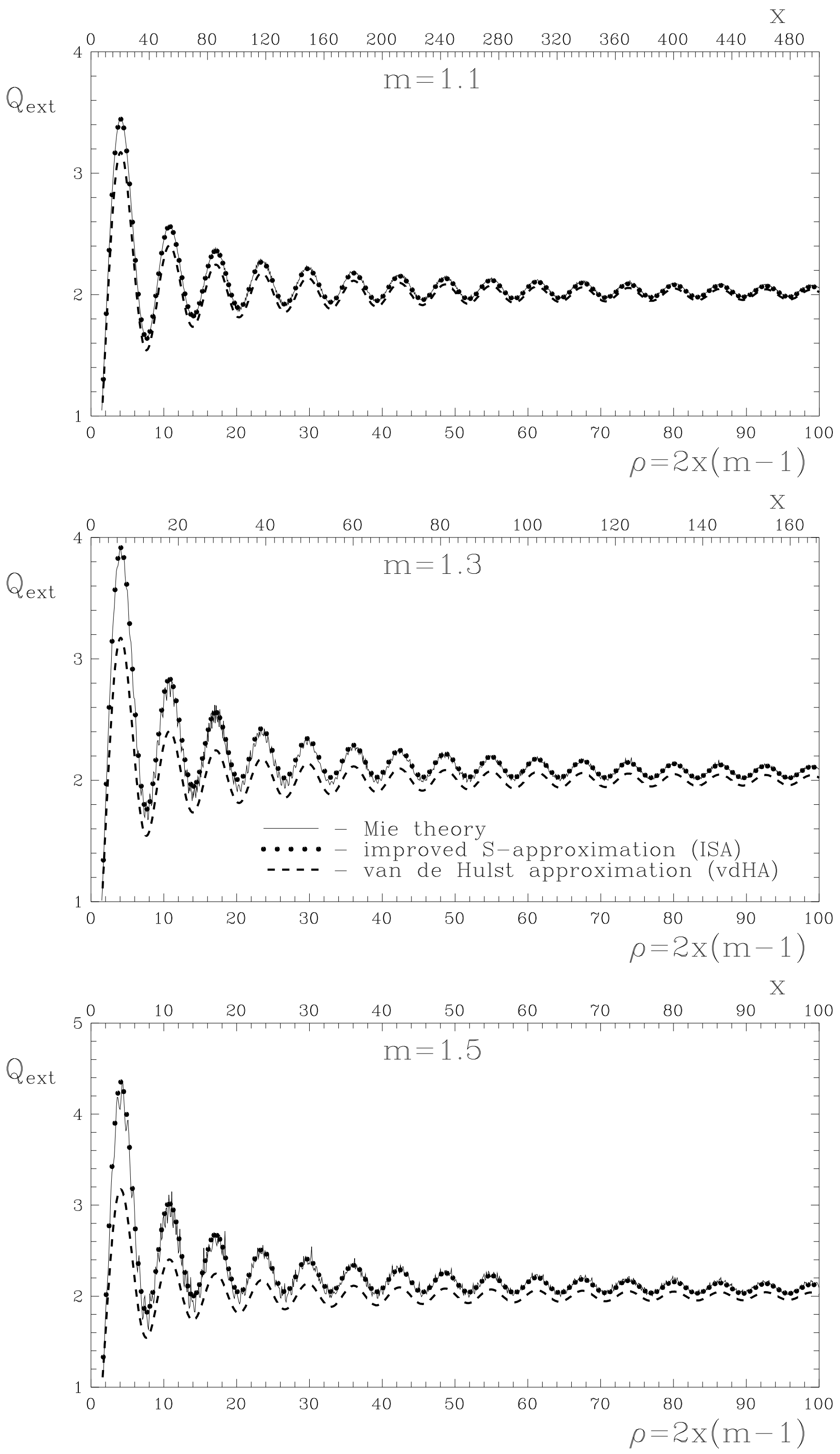

Fig. 2. Extinction efficiency factors calculated on the basis of Mie theory, improved S-approximation [Eqs. (29) – (31)], van de Hulst approximation [Eq. (1)], Rayleigh and Rayleigh-Gans approximations. The factors are plotted versus the phase shift ρ (lower x-axis) while the upper x-axis shows the corresponding size parameters x.

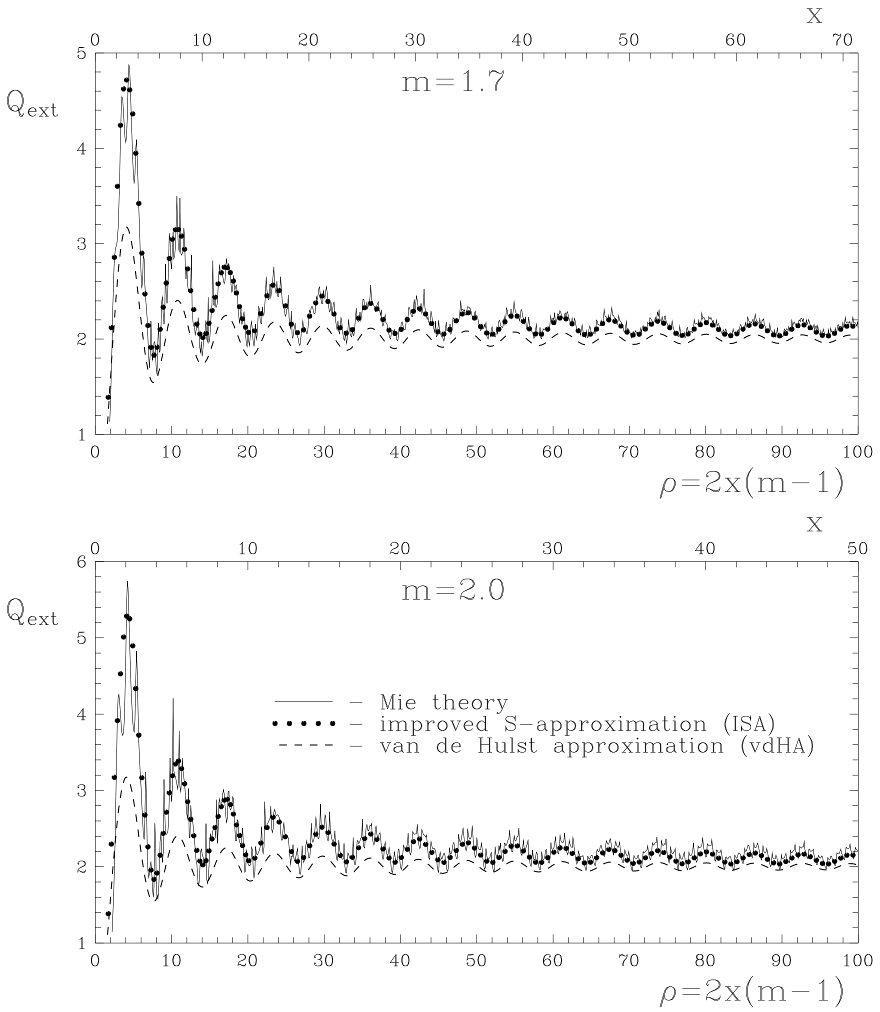

Fig. 2. (*continued.*)

It is seen that ε reduces when ρ increases and the ISA may be applied for the reliable representation of the extinction for particles with the refractive indices as large as 2.0 and more. But in these cases the fluctuations due to the ripple structure become very large and the deviations of the Mie curves from the "smoothed" ones given by the ISA may exceed several dozens of percents.

We also determined the range of validity of the ISA corresponding to the relative errors $|\varepsilon| \leq 1\,\%$, $5\,\%$ and $10\,\%$. The results presenting in Fig. 5 show the upper limits for the size parameter x in dependence on the refractive index m. They are plotted for the values of $m \geq m_*$ when the dependence of x on m may be approximated by the following power functions

$$x \lesssim 240\, m^{-15.6}\,, \qquad \text{if} \qquad |Q_{\rm ext}^{\rm ISA}/Q_{\rm ext}^{\rm Mie} - 1| \leq 1\%\,, \tag{33}$$

$$x \lesssim 160\, m^{-9.30}\,, \qquad \text{if} \qquad |Q_{\rm ext}^{\rm ISA}/Q_{\rm ext}^{\rm Mie} - 1| \leq 5\% \tag{34}$$

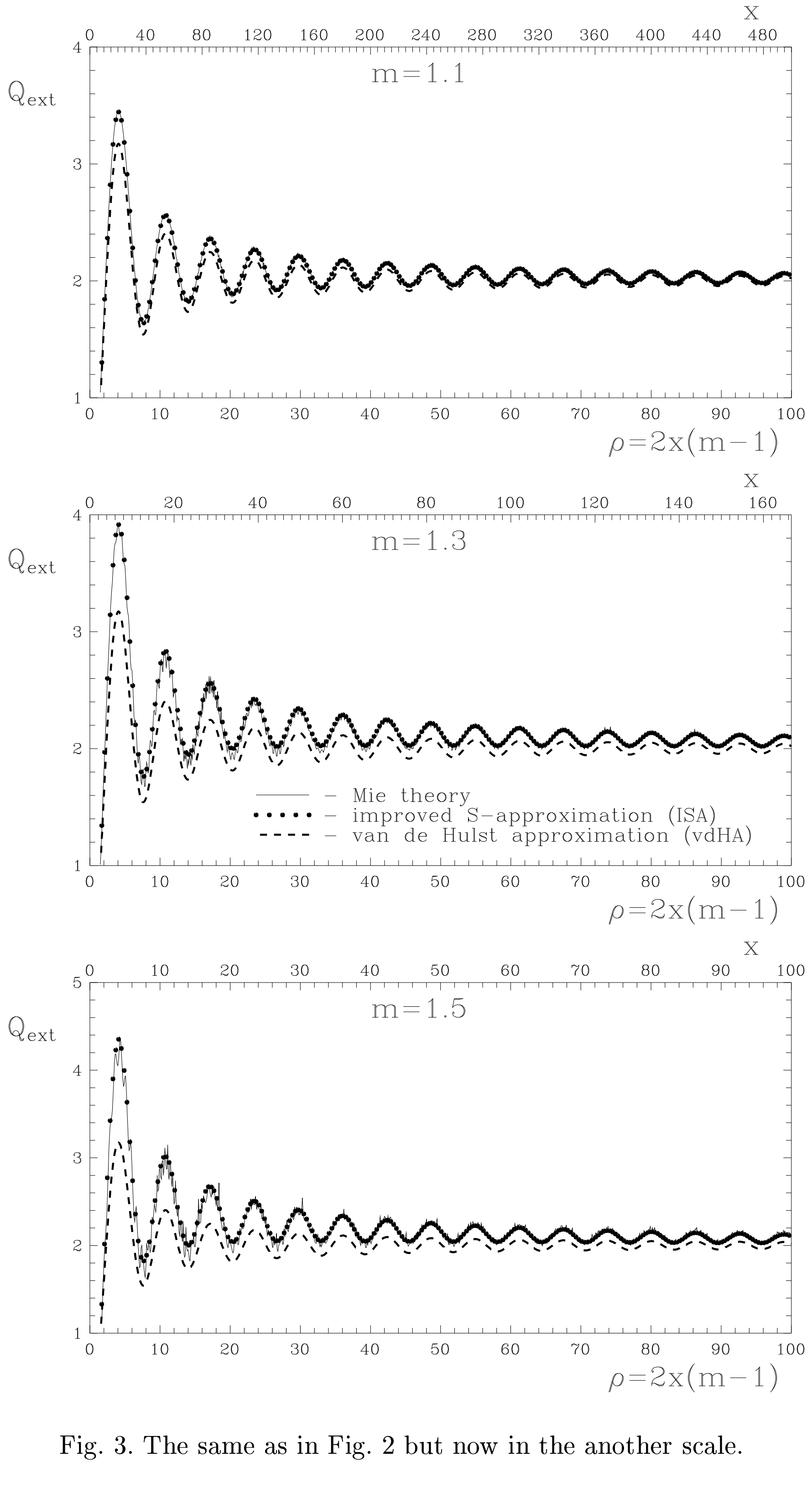

Fig. 3. The same as in Fig. 2 but now in the another scale.

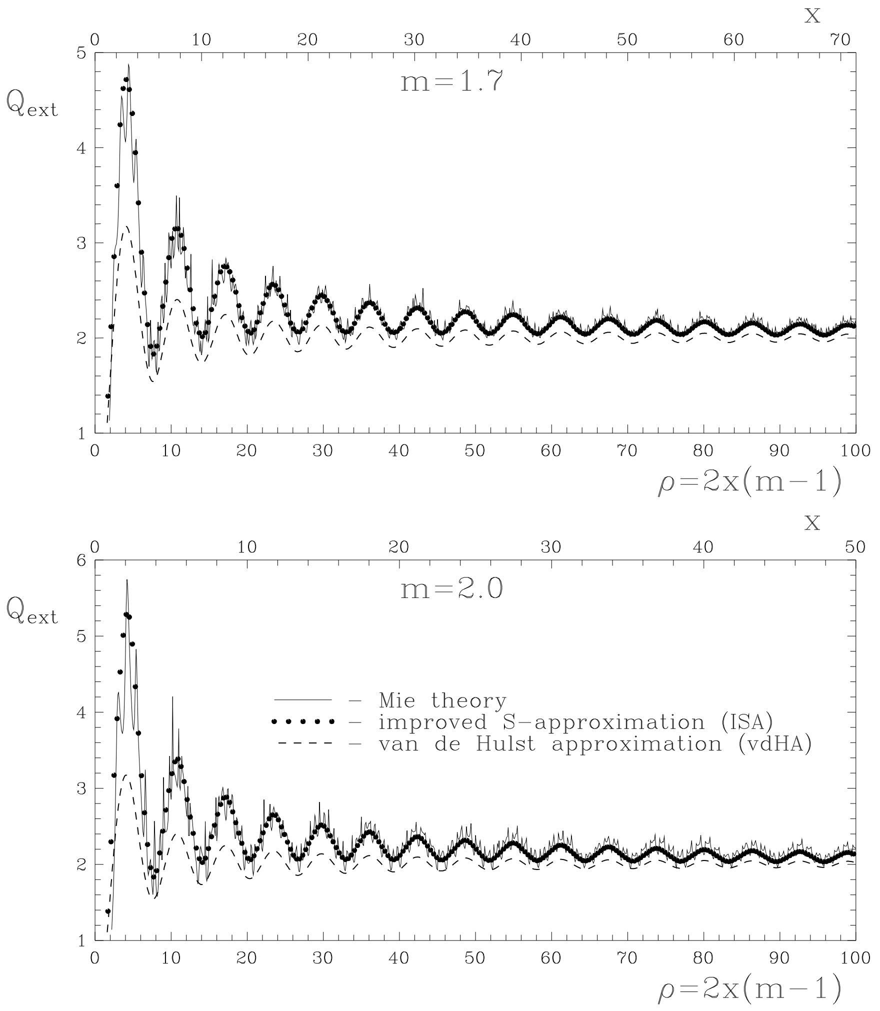

Fig. 3. (*continued.*)

and

$$x \lesssim 270\, m^{-9.99}\,, \qquad \text{if} \qquad |Q_{\rm ext}^{\rm ISA}/Q_{\rm ext}^{\rm Mie} - 1| \leq 10\%\,. \tag{35}$$

If $m < m_*$, the ISA may be used for arbitrarily large (infinite) values of x. This occurs for $m_* < 1.03$, $m_* < 1.10$ and $m_* < 1.22$ if the relative error being smaller than $1\,\%$, $5\,\%$ and $10\,\%$, respectively.

It should be noted that the S-approximation may be applied for the description of other optical characteristics besides extinction. It conserves the essential analytical properties of exact solution [see Eq. (23)]. On the contrary, both the van de Hulst and Rayleigh-Gans approximations are of different analytical structure as compared with the exact solution. At the same time, the known approximations of the Mie theory are derived starting from the S-approximation by the formal use of their validity conditions, and the role of each condition giving by Eqs. (20) and (21) can be explicitly shown. The

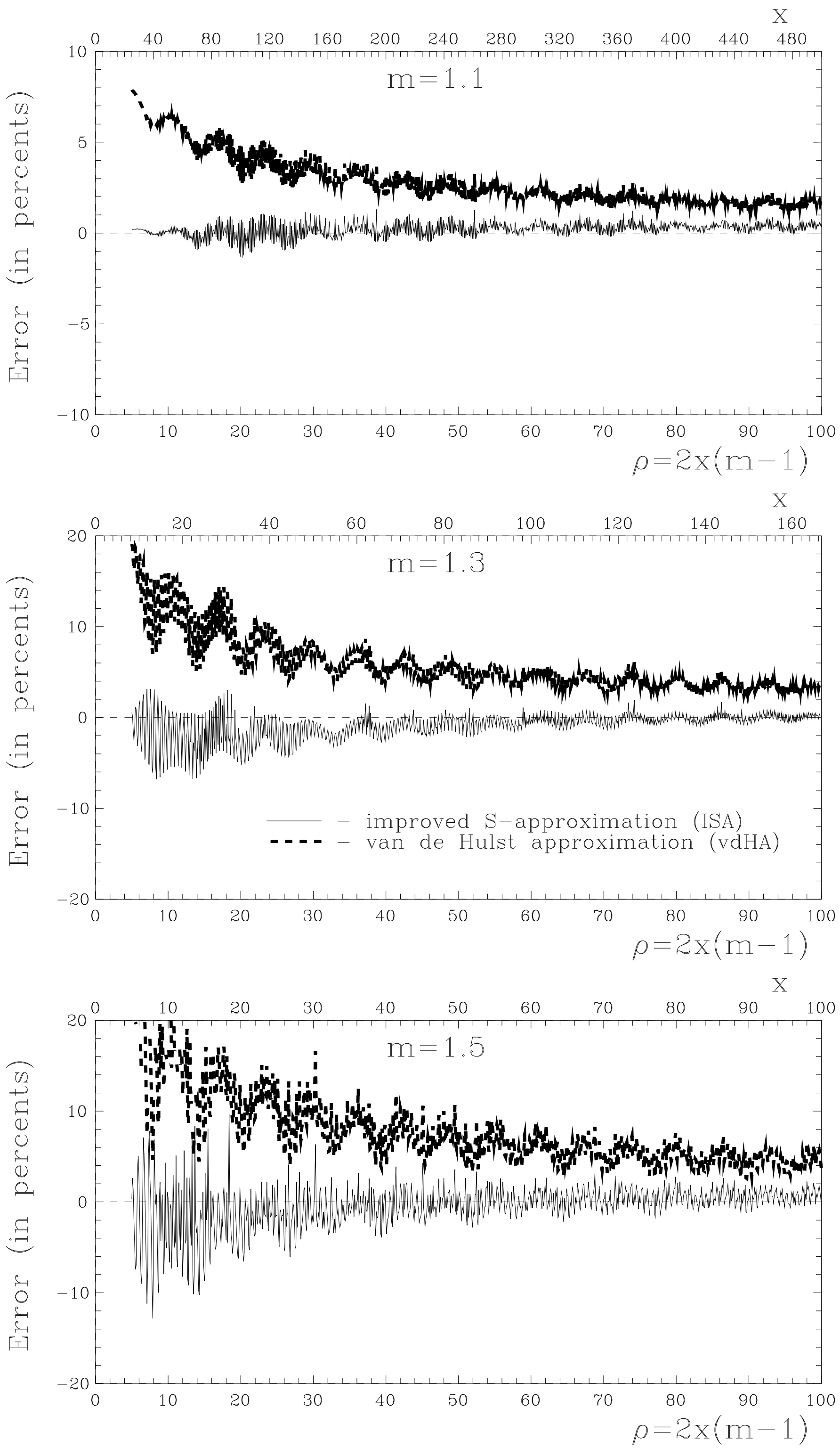

Fig. 4. Relative errors of calculations of the extinction efficiency factors in the case of improved S-approximation and van de Hulst approximation in the comparison with the Mie theory.

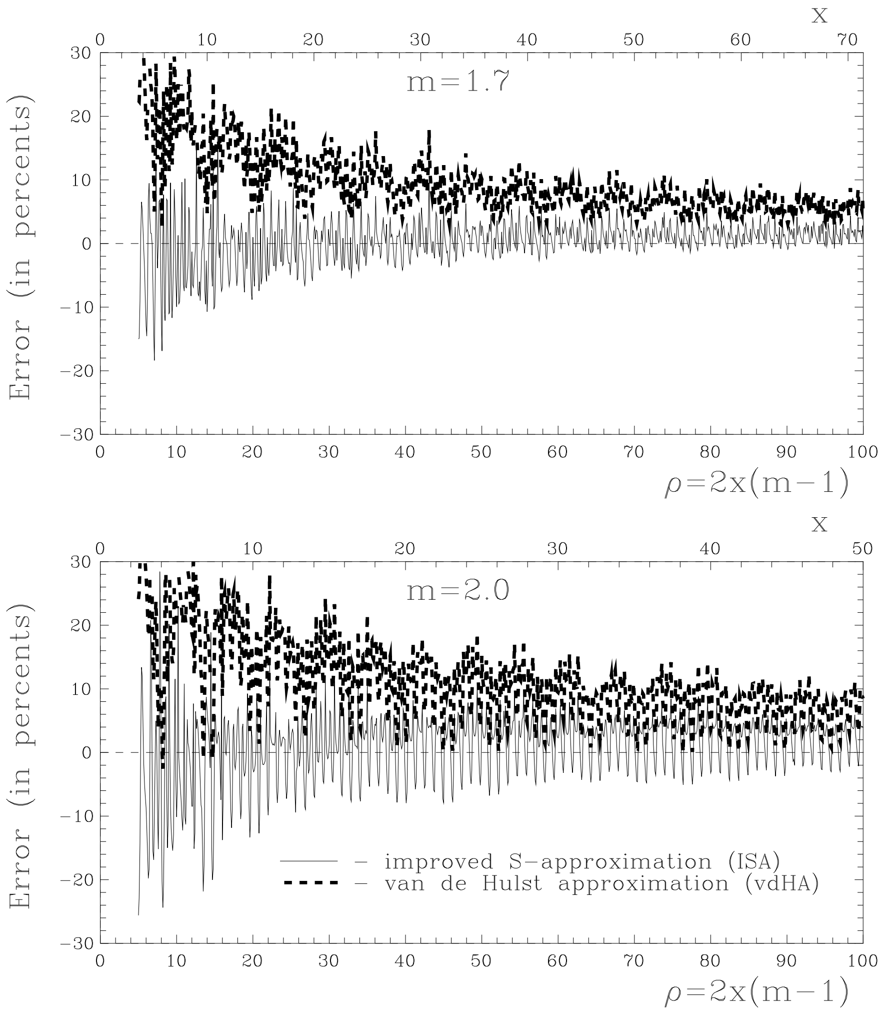

Fig. 4. (*continued.*)

analytical formulae of the S-approximation also open the wide opportunities for applications in solution to various direct and inverse problems.

4 Conclusions

We have considered the soft particles approximation (S-approximation) which reproduces the principal features of light scattering by large and soft spherical particles and its improved form (improved S-approximation) based on the correction for the short wavelength region. The S-approximation extends the results of the van de Hulst approximation of anomalous diffraction and may be used for calculations of the optical properties of particles with the refractive indices up to 2.0 and more.

Actually, the S-approximation restores the averaged curves of the Mie theory

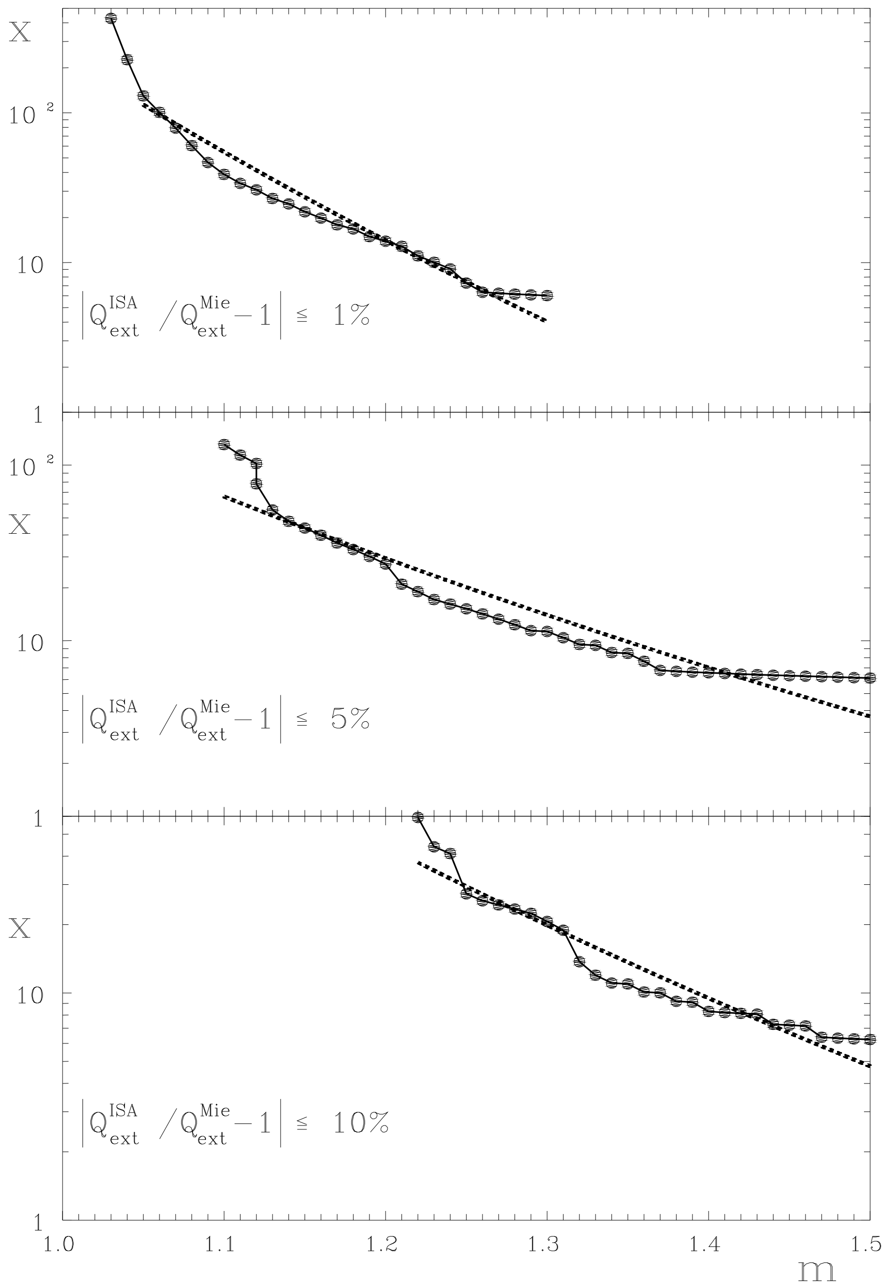

Fig. 5. Values of parameter x at which the efficiency factors in the improved S-approximation [Eqs. (29) – (31)] are calculated with different accuracy. The dashed curves show the power law approximations described by Eqs. (33) – (35).

without the appreciable errors (see Figs. 2, 3) and may be useful in order to get in the analytical form the "smoothed" Mie curves when the averaging of the ripple-type fluctuations was made.

The results obtained are of importance since the averaged characteristics are just used in a number of the direct and inverse optical problems.

Acknowledgements

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