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Notes

Far-field Lorenz–Mie scattering in an absorbing host medium. II: Improved stability of the numerical algorithm

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ABSTRACT

A recently developed FORTRAN program computing far-field optical observables for spherical particles in an absorbing medium has exhibited numerical instability arising when the product of the particle vacuum size parameter and the imaginary part of the refractive index of the host becomes sufficiently large. We offer a simple analytical explanation of this instability and propose a compact numerical algorithm for the stable computation of Lorenz–Mie coefficients based on an upward recursion formula for spherical Hankel functions of a complex argument. Extensive tests confirm an excellent accuracy of this algorithm approaching machine precision. The improved public-domain FORTRAN program is available at https://www.giss.nasa.gov/staff/mmishchenko/Lorenz-Mie.html.

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1. Introduction

Part I of this work [1] detailed the Lorenz–Mie theory of far-field electromagnetic scattering by a homogeneous spherical particle embedded in an unbounded absorbing host medium and described a public-domain FORTRAN program for the numerical computation of relevant optical observables. Subsequent massive computations for particle polydispersions have revealed that the program can fail when the product of the particle vacuum size parameter and the imaginary part of the refractive index of the surrounding medium becomes sufficiently large [2]. In this Part II we analyze the origin of this numerical instability and provide a simple remedy which makes the computer program stable over a wide range of scenarios relevant to actual practical applications.

2. Lorenz–Mie coefficients

Consistent with Ref. [1], we assume the $\exp(-\mathrm{i}\omega t)$ time-harmonic dependence of all electromagnetic fields, where $\mathrm{i} = (-1)^{1/2}$, ω is the angular frequency, and t is time. The dimensionless Lorenz–Mie coefficients a_n and b_n for a homogeneous spherical particle having a radius R are given by [1,3]

$$a_n = \frac{m^2 j_n(mx_1)[x_1 j_n(x_1)]' - j_n(x_1)[mx_1 j_n(mx_1)]'}{m^2 j_n(mx_1)\left[x_1 h_n^{(1)}(x_1)\right]' - h_n^{(1)}(x_1)[mx_1 j_n(mx_1)]'} \tag{1}$$

and

$$b_n = \frac{j_n(mx_1)[x_1 j_n(x_1)]' - j_n(x_1)[mx_1 j_n(mx_1)]'}{j_n(mx_1)\left[x_1 h_n^{(1)}(x_1)\right]' - h_n^{(1)}(x_1)[mx_1 j_n(mx_1)]'}, \tag{2}$$

where a prime indicates differentiation with respect to the corresponding argument in parentheses. Furthermore,

$$m = \frac{m_2}{m_1} = \frac{m'_2 + \mathrm{i}m''_2}{m'_1 + \mathrm{i}m''_1} \tag{3}$$

is the refractive index of the spherical particle (subscript "2") relative to that of the host medium (subscript "1");

$$x_1 = k_1 R \tag{4}$$

is the (generally complex-valued) size parameter of the particle; $j_n(z)$ are spherical Bessel functions of the first kind; and

$$h_n^{(1)}(z) = j_n(z) + \mathrm{i}y_n(z) \tag{5}$$

are spherical Hankel functions of the first kind, $y_n(z)$ being spherical Bessel functions of the second kind. The wave number of the host medium is given by

$$k_1 = k'_1 + \mathrm{i}k''_1 = \frac{2\pi m_1}{\lambda}, \tag{6}$$

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where λ is a vacuum wavelength. Note that

$$\omega = \frac{2\pi c}{\lambda}, \tag{7}$$

where c is the speed of light in a vacuum.

The numerical computation of the radial special functions entering Eqs. (1) and (2) can be highly non-trivial (see, e.g., Refs. [4,5] and numerous references therein). In Ref. [1] it is based on the following algorithm. The spherical Bessel functions of the first kind, $j_n(z)$ with $z = x_1$ or $z = mx_1$, obey the well-known recurrence relation [6,7]

$$j_{n+1}(z) = \frac{2n+1}{z} j_n(z) - j_{n-1}(z). \tag{8}$$

Since the upward recurrence is unstable, the standard practice is to define

$$r_n(z) = \frac{j_n(z)}{j_{n-1}(z)}, \tag{9}$$

which results in a stable downward recurrence formula

$$r_n(z) = \left[\frac{2n+1}{z} - r_{n+1}(z)\right]^{-1}. \tag{10}$$

If $n_{\max}$ is the largest order of the Lorenz–Mie coefficients, the downward recursion of Eq. (10) is initiated at $n = n_{\max} + n' \gg |z|$, where n' is an appropriately large number, using the starting value

$$r_{n_{\max}+n'}(z) \approx \frac{z}{2(n_{\max}+n')+1}. \tag{11}$$

The $j_n(z)$ are then computed using the straightforward upward recursion

$$j_n(z) = r_n(z) j_{n-1}(z), \quad n = 1, \ldots, n_{\max} \tag{12}$$

and the initial value

$$j_0(z) = \frac{\sin z}{z}. \tag{13}$$

The corresponding derivatives are computed using the recurrence relation

$$\frac{\mathrm{d}}{\mathrm{d}z}[z j_n(z)] = z j_{n-1}(z) - n j_n(z). \tag{14}$$

The computation of the Hankel functions (5) and their derivatives starts with the computation of the spherical Bessel functions of the first kind, as described above, followed by the computation of the spherical Bessel functions of the second kind using the upward recursion

$$y_{n+1}(z) = \frac{2n+1}{z} y_n(z) - y_{n-1}(z) \tag{15}$$

along with the initial values

$$y_0(z) = -\frac{\cos z}{z} \text{ and } y_1(z) = -\frac{\cos z}{z^2} - \frac{\sin z}{z}. \tag{16}$$

The corresponding derivatives follow from the recurrence formula

$$\frac{\mathrm{d}}{\mathrm{d}z}[z y_n(z)] = z y_{n-1}(z) - n y_n(z). \tag{17}$$

3. Numerical instability

Extensive double-precision FORTRAN computations have shown that when the product $k''_1 R$ becomes sufficiently large, the calculation of the spherical Hankel functions and their derivatives becomes unstable and eventually leads to zeros causing overflows in the Lorenz–Mie coefficients (1) and (2). Running the same FORTRAN program in extended precision (e.g., using the `-freal-8-real-16` compilation option in GFortran) serves to increase the "stable" range of $k''_1 R$ values, but eventually the instability reoccurs. Although this happens for m''_1 values that are likely too large to consider in the context of far-field scattering (i.e., when strong absorption in the host medium is expected to virtually eradicate any optical observable), it is still important to understand the origin of this problem and find a stable practical solution. This is done in the following two sections.

4. Origin of numerical instability

A simple analysis helps attribute the identified numerical instability to the use of the representation (5) in combination with the separate computation of the spherical Bessel functions $j_n(k_1R)$ and $y_n(k_1R)$. Indeed, in the limit $|k_1R| \to \infty$, we have the following asymptotic expressions [6,7]:

$$\begin{aligned} j_n(k_1R) = {} & \frac{1}{2\mathrm{i}k_1R} \exp\left[\mathrm{i}\left(k_1R - \tfrac{1}{2}n\pi\right)\right] \\ & - \frac{1}{2\mathrm{i}k_1R} \exp\left[-\mathrm{i}\left(k_1R - \tfrac{1}{2}n\pi\right)\right] \\ & + \exp\left(k''_1 R\right) O\left[(k_1R)^{-2}\right], \end{aligned} \tag{18}$$

$$\begin{aligned} \mathrm{i}y_n(k_1R) = {} & \frac{1}{2\mathrm{i}k_1R} \exp\left[\mathrm{i}\left(k_1R - \tfrac{1}{2}n\pi\right)\right] \\ & + \frac{1}{2\mathrm{i}k_1R} \exp\left[-\mathrm{i}\left(k_1R - \tfrac{1}{2}n\pi\right)\right] \\ & + \exp\left(k''_1 R\right) O\left[(k_1R)^{-2}\right], \end{aligned} \tag{19}$$

and

$$h_n^{(1)}(k_1R) \sim \frac{1}{\mathrm{i}k_1R} \exp\left[\mathrm{i}\left(k_1R - \tfrac{1}{2}n\pi\right)\right]. \tag{20}$$

These expressions imply that computing $h_n^{(1)}(k_1R)$ according to Eq. (5) can become highly problematic if $k''_1 R$ is sufficiently large. Indeed, then the second and third terms in either Eq. (18) or (19) can dwarf the first term to such an extent that adding the latter does not change the sum of the second and third terms to machine precision (i.e., 15–17 decimal digits in the double-precision FORTRAN representation). Yet it is the first terms in Eqs. (18) and (19) that define the value of $h_n^{(1)}(k_1R)$. As a consequence, adding $j_n(k_1R)$ and $\mathrm{i}y_n(k_1R)$ can lead to large round-off errors. Furthermore, if $\mathrm{i}y_n(k_1R) = -j_n(k_1R)$ to machine precision then $h_n^{(1)}(k_1R)$ vanishes. The use of

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}(k_1R)}\left[k_1R h_n^{(1)}(k_1R)\right] = {} & \frac{\mathrm{d}}{\mathrm{d}(k_1R)}[k_1R j_n(k_1R)] \\ & + \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}(k_1R)}[k_1R y_n(k_1R)] \end{aligned} \tag{21}$$

along with Eqs. (14) and (17) can cause the same numerical problem. As a result, the entire denominator in either Eq. (1) or (2) can vanish, thereby causing overflows.

It should be noted that this instability is not exclusive to the algorithm described in Ref. [1] but is relevant to other commonly used Lorenz–Mie algorithms, including that by Bohren and Huffman (see Appendix B of Ref. [8]).

5. Stable numerical scheme

Massive computer calculations have demonstrated that a remarkably simple and straightforward resolution of the above numerical instability problem is to abandon Eqs. (5) and (21) and compute the spherical Hankel functions using the upward recursion

$$h_{n+1}^{(1)}(z) = \frac{2n+1}{z} h_n^{(1)}(z) - h_{n-1}^{(1)}(z) \tag{22}$$

(see Refs. [6,7]) in combination with the initial values

$$h_0^{(1)}(z) = -\frac{\mathrm{i}\exp(\mathrm{i}z)}{z} \tag{23}$$

and

$$h_1^{(1)}(z) = -\frac{\exp(\mathrm{i}z)(z+\mathrm{i})}{z^2}. \tag{24}$$

The corresponding derivative is then computed according to

$$\frac{\mathrm{d}}{\mathrm{d}z}\left[zh_n^{(1)}(z)\right] = zh_{n-1}^{(1)}(z) - nh_n^{(1)}(z). \tag{25}$$

The Bessel functions of the first kind $j_n(x_1)$ and $j_n(mx_1)$ as well as their derivatives entering Eqs. (1) and (2) are still computed using the stable downward recursion (10), while the computation of the Bessel functions of the second kind $y_n(x_1)$ is avoided altogether.

Note that the upward recursion (22) for $h_n^{(1)}(z)$ is known to cause minor issues for a real-valued z (or that with a very small imaginary part) [9]. In particular, the real part of $h_n^{(1)}(z)$, i.e., $j_n(z)$, can be calculated with very poor *relative* accuracy if $n > z$. However, the error in the real part is still much smaller than the absolute value of $h_n^{(1)}(z)$; more specifically, the ratio of the former to the latter does not significantly exceed machine epsilon. Since the imaginary part of $h_n^{(1)}(z)$, i.e., $y_n(z)$, never vanishes in this range of z, a high accuracy of computing the overall value of $h_n^{(1)}(z)$ (i.e., without separation into the real and imaginary parts) is guaranteed by this algorithm for an arbitrary n and any z with a non-negative imaginary part.

Extensive numerical checks of the new program have revealed no instability in double-precision FORTRAN computations even for $k''_1 R$ values as large as 350. A compelling test has been to run the same program using the extended-precision compilation option, which has demonstrated excellent agreement with the original double-precision output. This is illustrated by the Lorenz–Mie coefficients computed for the following model: the vacuum wavelength is $\lambda = 2\pi\,\mu$m; the radius of the particle is $R = 2500\,\mu$m; and the refractive indices of the host medium and of the particle material are $m_1 = 1.33 + \mathrm{i}0.1$ and $m_2 = 1$, respectively. For $n = 1$, the double-precision result is

$$\begin{aligned} a_1 = {} & (4.3914709187499176\mathrm{D}+216, \\ & -6.1540139314269924\mathrm{D}+216), \end{aligned} \tag{26}$$

$$\begin{aligned} b_1 = {} & (6.0677381984696521\mathrm{D}+216, \\ & -2.4794566280970265\mathrm{D}+216), \end{aligned} \tag{27}$$

while the corresponding extended-precision output is

$$\begin{aligned} a_1 = {} & (4.3914709187514217915479323919636935 3\mathrm{Q}+216, \\ & -6.1540139314259443653772427032760145 4\mathrm{Q}+216), \end{aligned} \tag{28}$$

$$\begin{aligned} b_1 = {} & (6.0677381984702483911710220609406386 0\mathrm{Q}+216, \\ & -2.4794566280956997211740745112390984 2\mathrm{Q}+216). \end{aligned} \tag{29}$$

For $n = 3402$, the respective double-precision and extended-precision results are

$$\begin{aligned} a_{3402} = {} & (6.5263656298271867\mathrm{D}+20, \\ & -1.0743959632382240\mathrm{D}+21) \end{aligned} \tag{30}$$

$$\begin{aligned} b_{3402} = {} & (6.2207616536588911\mathrm{D}+20, \\ & -5.3211289141292931\mathrm{D}+20) \end{aligned} \tag{31}$$

Table 1
Extinction efficiency factor as a function of m''_1 and x.

x	Q_{ext} ($m''_1 = 10^{-5}$)	Q_{ext} ($m''_1 = 0.01$)	Q_{ext} ($m''_1 = 0.06$)
0.5	−0.133333D−04	−0.133444D−01	−0.804769D−01
5	−0.133338D−03	−0.138159D+00	−0.100002D+01
50	−0.133383D−02	−0.199948D+01	−0.222396D+03
500	−0.133835D−01	−0.792769D+04	−0.749013D+25
5000	−0.138469D+00	−0.106451D+43	−0.251250D+259

and

$$\begin{aligned} a_{3402} = {} & (6.5263656298272348588623574929279220 7\mathrm{Q}+20, \\ & -1.0743959632381830957828310329342402 8\mathrm{Q}+21), \end{aligned} \tag{32}$$

$$\begin{aligned} b_{3402} = {} & (6.2207616536588383364649276671198913 4\mathrm{Q}+20, \\ & -5.3211289141290276620227222272159417 6\mathrm{Q}+20). \end{aligned} \tag{33}$$

Both the double-precision and the extended-precision runs yielded the same extinction cross section $C_{\mathrm{ext}} = 0.388777 \times 10^{222}\,\mu\mathrm{m}^2$. However, the extended-precision value of the effective scattering cross section, $C_{\mathrm{sca}}^{\mathrm{eff}} = 0.777958 \times 10^{439}\,\mu\mathrm{m}^2$, was outside the range of double-precision floating-point FORTRAN representation of real numbers (from 10^{-308} to 10^{308}). The double-precision computation of the corresponding scattering matrix was also impossible for the same reason.

Our computations have shown that extremely large $k''_1 R$ values can eventually cause the real and/or imaginary parts of the Lorenz–Mie coefficients a_n and b_n to exceed, in absolute value, the double-precision floating-point FORTRAN limit of 10^{308}. This is a separate problem that must be addressed specifically, including the practical aspect of the subsequent computation of relevant optical observables from such large Lorenz–Mie coefficients. The commonly used logarithmic derivatives of the Riccati–Bessel functions [8,9] would not resolve this issue because it is not the intermediate function values but the final coefficients and subsequent optical observables that become too large. The only ultimate fix would be to isolate the main order of this magnitude analytically. Perhaps the simplest, albeit not necessarily cost-effective, practical solution is to run the FORTRAN program in the extended-precision mode with its 10^{4932} floating-point limit. Fortunately, such excessively large $k''_1 R$ values are very unlikely to be encountered in actual far-field scattering applications.

6. Numerical example

To illustrate the performance of the resulting FORTRAN program, Table 1 lists the values of the extinction efficiency factor $Q_{\mathrm{ext}} = C_{\mathrm{ext}}/(\pi R^2)$ computed with double precision for several discrete values of m''_1 and the vacuum size parameter $x = 2\pi R/\lambda$ assuming that $m'_1 = m_2 = 1.3$. One can see that *all* the tabulated Q_{ext} values are negative, which may seem to be inconsistent with the findings previously reported in Refs. [2,10]. Yet this remarkable result is perfectly in line with (i) the notion of the extinction cross section as quantifying the difference between the readings of a forward-scattering detector of light in the absence of the particle and with the particle present, and (ii) the explanation of extinction as being the result of interference of the incident and forward-scattered fields [11]. Indeed, since $m'_1 = m_2$, the field directly transmitted by the particle accumulates no path-length phase shift and arrives at the forward-scattering detector in phase with the incident field. Furthermore, unlike the incident field, the directly transmitted field does not experience exponential attenuation over the

corresponding path lengths inside the particle. As a consequence, the signal recorded by the detector can be expected to rapidly grow with particle size, implying negative extinction with rapidly growing magnitude. The growth in Q_{ext} is approximately linear for $m''_1 = 10^{-5}$, implying that the negative differential absorption (i.e., "lost absorption") inside the particle is proportional to the particle volume. For the larger values of m''_1, the exponential character of the negative differential attenuation becomes much more pronounced.

7. Concluding remarks

In summary, we have described a simple and accurate way to compute the Lorenz–Mie coefficients for spherical particles immersed in an unbounded absorbing host. Unlike the previous version of the algorithm, the new numerical scheme is based on a direct calculation of the spherical Hankel functions $h_n^{(1)}(z)$ of a complex-valued argument using the upward recursion of Eq. (22). A convenient ingredient of this recursion scheme is the possibility to explicitly factor out $\exp(\mathrm{i}z)$ in the starting values of $h_0^{(1)}(z)$ and $h_1^{(1)}(z)$ (Eqs. (23) and (24)). Extensive tests have demonstrated an excellent stability of this scheme and numerical accuracy approaching machine precision.

These results may also be useful in the context of the Lorenz–Mie theory for concentric layered spheres in which some layers are made of absorbing materials [5,8]. This is not surprising since a core–mantle sphere with a very large size of the absorbing mantle is a physically appropriate model for the infinite absorbing host medium [12].

The new double-precision FORTRAN program is in the public domain and can be accessed at https://www.giss.nasa.gov/staff/mmishchenko/Lorenz-Mie.html. Based on the test runs described in Sections 5 and 6, we expect it to be applicable and highly accurate as long as the Lorenz–Mie coefficients and the corresponding optical observables do not cause overflows by exceeding the double-precision floating-point FORTRAN limit of 10^{308}. Should such overflows occur, the simplest workable solution would be to run the same program in the extended-precision mode.

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