LOGARITHMIC DERIVATIVE OF THE RICCATI–BESSEL FUNCTIONS OF THE FIRST KIND IN CALCULATIONS BY THE MIE THEORY

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Accuracy criteria for calculation of the logarithmic derivative A_n of the Riccati–Bessel function of the first kind by the Mie theory are proposed. A combined algorithm for calculation of A_n is described. It allows one to reduce the capacity of a random–access memory thereby providing the opportunity for calculating the optical characteristics of particles with a diffraction parameter of 10^6 and larger using a PC.

1. INTRODUCTION

Results of numerical study of the optical characteristics of aerosol particles by the Mie theory are widely used in ecology for investigation of dispersed atmospheric and water polluttants; in astrophysics for diagnostics of the properties of interstellar matter and the atmospheres of planets and comets; in microbiology, chemistry, and polymeric technology for determination of the size and concentration of macromolecular structures; and, in plasma physics and optics for determination of the parameters of inhomogeneities.[1–4] The central problem associated with such calculations is determination of the logarithmic derivative A_n of the Riccati–Bessel functions of the first kind of the complex argument $z = r + i\mu$ (Ref. 5).

In this paper the well–known methods for calculating A_n are compared and accuracy criteria are proposed. New method for calculating A_n allows one to reduce the capacity of a random–access memory and to decrease somewhat the execution time. In addition, for the first time the optical characteristics of the particle with a diffraction parameter of 10^6 and larger can be calculated using personal computers.

The use of logarithmic derivative A_n of the Riccati–Bessel functions of the first kind (RBF1) considerably extends the range of applicability of numerical investigations by the Mie theory with the help of a modern PC. To calculate the terms A_n, backward recursion is commonly used of the following form:[6–8]

$$A_{n-1} = \frac{n}{z} - \frac{1}{A_n + \frac{n}{z}} . \qquad (1.1)$$

In this case the calculation starts from a certain number $N > |z|$ for which it is assumed that[6,7]

$$A_N = 0 . \qquad (1.2)$$

Assumption (1.2) contradicts the asymptotic behavior of A_n which has the form[6]

$$A_N \simeq (N + 1)\, z^{-1} \qquad (1.3)$$

and points to a considerable increase in A_n as n increases. In spite of this fact, substitution of Eq. (1.2) into Eq. (1.1) makes it possible to find the correct terms A_n for $n = 1, 2, \ldots, l$, where the quantity l is slightly less than an initial number N from which we started to calculate the sequence A_n. This is provided by the absolute stability of a procedure for calculating by Eq. (1.1) (see Ref. 6). The necessity of holding of all the calculated terms A_n in the random–access memory can be considered as a disadvantage of this procedure. Moreover, the length l of the correctly calculated subsequence A_n should be sufficient for the Mie series summation.

The lack of methods for estimating the accuracy of calculation of A_n eliminates the possibility of real–time control over the Mie series convergence within the length l of the correctly calculated sequence. In this paper we study the potentialities of forward recursion. The advisability of the A_n calculation from the corresponding continued fraction for $n \geq 0.3|z| + 1$ is shown. A combined algorithm for calculating A_n is developed without holding of the entire array A_n in the random–access memory except for one or two current values. As a result, there appears a possibility to perform calculations by the Mie theory using personal computers consuming for this purpose not more than 50 Kbytes of the random–access main memory independently of the values of the diffraction parameter of a particle (up to 10^6 and larger) and the light absorption coefficient of particle material.

2. ACCURACY CRITERIA FOR THE CALCULATION OF A_n

Calculations by Eqs. (1.1) and (1.2) yield the sequence A_n, $n = 1, 2, \ldots, N$, first terms ($n = 1, 2, \ldots, l$) are calculated correctly but the last terms ($n = l + 1, \ldots, N$) are characterized by the inadmissibly large error. The value of l is estimated, as a rule, intuitively because there are no accuracy criteria for calculating the sequence A_n. At the same time such criteria can be obtained from the relations of the Riccati–Bessel functions of the first φ_n, the second χ_n, and the third ξ_n kinds[9,10]

$$\xi_n \varphi_n' - \xi_n' \varphi_n = i , \qquad (2.1)$$

$$\varphi_n \chi_{n-1} - \varphi_{n-1} \chi_n = z^{-4} , \qquad (2.2)$$

$$\varphi_{n+1} \chi_{n-1} - \varphi_{n-1} \chi_{n+1} = \frac{2n + 1}{z^5} . \qquad (2.3)$$

The derivatives φ_n' and ξ_n' (z) are defined by the relation of the following form[10]:

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$$f'_n = f_{n-1} - \frac{n}{z} f_n \,. \tag{2.4}$$

By substituting Eq. (2.4) into the formula for logarithmic derivative of the RBF1 (see Ref. 5)

$$A_n = \varphi'_n \varphi_n^{-1} \,, \tag{2.5}$$

we derive

$$A_n = \varphi_{n-1} \varphi_n^{-1} - \frac{n}{z} \,. \tag{2.6}$$

Let us write down relations (2.1)–(2.3) in the form

$$\frac{\xi_n \varphi'_n - \xi'_n \varphi_n}{\xi_{n-1} \varphi'_{n-1} - \xi'_{n-1} \varphi_{n-1}} = 1 \,, \tag{2.7}$$

$$\frac{\varphi_n \chi_{n-1} - \varphi_{n-1} \chi_n}{\varphi_{n-1} \chi_{n-2} - \varphi_{n-2} \chi_{n-1}} = 1 \,, \tag{2.8}$$

$$\frac{\varphi_{n+1} \chi_{n-1} - \varphi_{n-1} \chi_{n+1}}{\varphi_{n+2} \chi_n - \varphi_{n+2} \chi_n} = \frac{2n+1}{2n+3} \,. \tag{2.9}$$

By substituting Eq. (2.6) into Eqs. (2.7)–(2.9) and using the relations for the RBF1 (see Ref. 10)

$$\varphi_{n+2} = \frac{2n+3}{z} \varphi_{n+1} - \varphi_n \,, \tag{2.10}$$

we obtain the following equations:

$$F_1(l) = A_l \, (\xi_l - A_{l-1} \xi_{l-1} + \xi'_{l-1}) -$$

$$- \frac{l}{z} A_{l-1} \xi_{l-1} - \xi'_l + \xi'_{l-1} \frac{l}{z} \,, \tag{2.11}$$

$$F_2(l) = \left(A_l + \frac{l}{z} \right)^{-1} \chi_{l-1} - \chi_l - \chi_{l+2} + \left(A_{l-1} + \frac{l-1}{z} \right) \chi_{l-1}, \tag{2.12}$$

$$F_3(l) = \frac{\chi_{l-1} - \left(A_l + \frac{l}{z} \right) \left(A_{l+1} + \frac{l+1}{z} \right) \chi_{l+1}}{\frac{2l+3}{z} \chi_l - (\chi_l + \chi_{l+2}) \left(A_{l+1} + \frac{l+1}{z} \right)} - \frac{2l+1}{2l+3}. \tag{2.13}$$

The accuracy criterion in calculating the spherical functions and A_n is the proximity to zero of the functions $F_1(l)$, $F_2(l)$, and $F_3(l)$.

One more accuracy criterion of the $A_n(z)$ calculation is the relation derived from Eqs. (2.5) and (2.6)

$$F_4(n) = A_n - (\alpha(z) - n) \, z^{-1} \,, \tag{2.14}$$

where $\alpha(z)$ is the continued fraction of the form[11]

$$\alpha(z) = 2n + 1 - \cfrac{z^2}{2n + 3 - \cfrac{z^2}{2n + 5 - \cfrac{z^2}{\cdots}}} \,, \tag{2.15}$$

which is equal to the RBF1 ratio of the form[11]

$$\alpha(z) = z \frac{\varphi_{n-1}}{\varphi_n} \,. \tag{2.16}$$

The procedure for the $\alpha(z)$ calculation is discussed below. A sharp increase in $F_1(l)$, ..., $F_4(l)$ as l increases indicates possible inadmissible growth of the error. The terms $F_1(l)$, ..., $F_4(l)$ of the sequence A_n calculated from Eqs. (1.1)–(1.3) for $z = 10 - i\,10$ beginning with $N = 40$ showed the following fact. Quadruple–precision complex numbers instead of single–precision ones do not increase the rate of convergence of a monotonically decreasing sequence. In the case under consideration the change–over from Eq. (1.2) to Eq. (1.3) results in one–step increment in the length l of the sequence $A_n(z)$ calculated to three significant digits beyond the decimal point. When using Eq. (1.2), $l = 37$ and for Eq. (1.3) $l = 38$. With increase in the modulus of the imaginary part of z the deviation from zero of the initial terms $F_1(l)$, ..., $F_4(l)$ increases. The change–over from the single–precision numbers to quadruple ones ensures a decrease in the modula of the initial terms $F_1(l)$, ..., $F_4(l)$. Thus the calculations by backward recursion should be preferably started from the asymptotic value of A_n but not from zero. The length of the correctly calculated sequence can be determined from Eqs. (2.11)–(2.14).

3. CALCULATION OF THE SEQUENCE OF THE RBF1 LOGARITHMIC DERIVATIVE BY FORWARD RECURSION

The RBF1 logarithmic derivative is calculated by the formula

$$A_n = -\frac{n}{z} + \left[\frac{n}{z} - A_{n-1} \right]^{-1} \,. \tag{3.1}$$

The initial value of $A_0(z)$ being substituted into Eq. (3.1) to start the calculations of $A_n(z)$ is equal to[5–7]

$$A_0 = \cot z \,. \tag{3.2}$$

The formula for cotangent of the complex number has the following form[6]

$$\cot z = \frac{\sin(r) \cos(r) + i \sinh(\mathrm{m}) \cosh(\mathrm{m})}{\sin^2(r) \sinh^2(\mathrm{m})} \,.$$

For large values of μ it is advisable to use the asymptotic formula for cotangent

$$A_0 = \begin{cases} (0, i), \text{ for } \mu \le -\beta, \\ (0, -i), \text{ for } \mu \ge \beta, \end{cases} \tag{3.3}$$

instead of Eq. (3.2) to avoid the errors due to exponent overflow. Here $\beta \approx 170$. However, the quantity A_0 becomes equal to its asymptotic value (3.3) for $\beta \ll 170$. This is achieved the faster, the shorter is the real number length. Therefore, the optimal choice of the value β at which relation (3.3) starts to be valid depends on the length of real and complex numbers. In the case of single–precision number (*real**4 and *complex**8) it is preferable to choose $\beta \approx 8.08$, for number (*real**8 and *complex**16) $\beta = 17.3$, and for the quadruple–precision number (*real**16 and *complex**32) $\beta \approx 37.4$. Calculations by forward recursion

(3.1) enable us to avoid holding of all the values of A_n in the random–access memory except for two last ones. This advantage incurs a risk of accumulated errors characteristic of Eq. (3.1).

Calculations by Eq. (3.1) result in significant errors for $n \gtrsim |z|$ (see Refs. 5–7). This fact is responsible for the errors in calculating the efficiency factors for metal particles with the diffraction parameter $\ldots \kappa\rho \ldots > 30$ by the Mie theory (see Ref. 5). The step at which an error creeps in the sequence A_n depends on the length of the machine number. Figure 1 illustrates the results of calculation of the sequences $\mathrm{Re}\{A_n\}$ (curves *2*, *4*, *6*, and *8*) and $\mathrm{Im}\{A_n\}$ (curves *1*, *3*, *5*, and *7*) for $z = (10 - i\,10)$ with the single–precision (curves *7* and *8*), double–precision (curves *5* and *6*), and quadruple–precision numbers (curves *3* and *4*). For small n all the results of calculations of A_n are in a good agreement. As n increases, accumulation of errors characteristic of monotonically increased sequence results in an inadmissibly large error in calculations with the single–precision numbers (curves *7* and *8*) beginning from $l_1 = 15$. The double–precision numbers used to find the sequence A_n by Eq. (3.1) for $z = 10 - i\,10$ yield the correct results up to $l_2 = 24$, while the quadruple–precision numbers up to $l_3 = 38$.

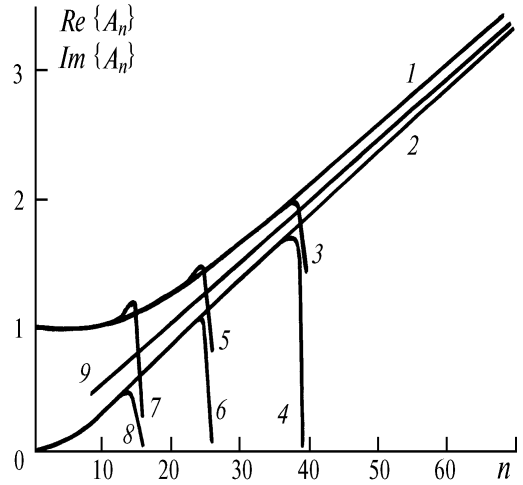

FIG. 1. The sequences $\mathrm{Re}\{A_n\}$ *(curves 2, 4, 6, 8, and 9) and* $\mathrm{Im}\{A_n\}$ *(curves 1, 3, 5, 7, and 9) for* $z = (10 - i\,10)$ *for the single–precision (curves 7 and 8), double–precision (curves 5 and 6), and quadruple–precision numbers (curves 3 and 4) calculated by forward recursion (3.1). Curves 1 and 2 are calculated from continued fraction* [*see Eq. (4.1)*]. *Straight line 9 shows the asymptotic estimate of* $\mathrm{Re}\{A_n\}$ *and* $\mathrm{Im}\{A_n\}$.

Figures 2*a* and *b* show the results of calculation of l_1, l_2, and l_3 as functions of the real r and imaginary parts of the complex argument $z = r + i\,\mu$. In Fig. 2*a* the modula of the negative quantities μ are plotted along the y axis. Let us denote the variable part of the argument z by x (in Fig. 2*a* it is r, in Fig. 2*b* it is $|\mu|$), and the parameter of the argument by p ($|\mu|$ in Fig. 2*a* and r in Fig. 2*b*). It is clear from Fig. 2 that for $x \le p$ the quantities l_1, l_2, and l_3 depend on p rather than x

$$l_1 \approx 2|p| + 2 ,$$

$$l_2 \approx 4|p| + 4 ,$$

$$l_3 \approx 6|p| + 6 .$$

The only exception is the region of minimum of $l_1 - l_3$ for $\mu \in (10, 100)$. For $x > p$ the dependence of the quantity $l_1 - l_3$ on the parameter p disappears. From Fig. 2 one can see that for large x all the curves l_1, l_2, and l_3 tend to merge into three groups.

4. USE OF CONTINUED FRACTION TO DETERMINE A_n

By substituting Eqs. (2.15) and (2.16) into Eq. (2.6) we derive the following relation:

$$A_n = (\alpha(z) - n)\, z^{-1} , \tag{4.1}$$

which can be used for calculating the quantity A_n for $k < n$ without holding of the preceding values of A_n in the random–access memory (see Ref. 7). Two algorithms for calculating the continued fractions are familiar, namely, forward recursion (FR) and backward recursion (BR) algorithms (see Ref. 12). As applied to Eq. (2.15), the FR algorithm can be written as follows:

$$b_\kappa = 2n + 2\kappa + 1 ,$$

$$P_\kappa = b_\kappa P_{\kappa-1} - z^2 P_{\kappa-2} ,$$

$$Q_\kappa = b_\kappa Q_{\kappa-1} - z^2 Q_{\kappa-2} , \tag{4.2}$$

$$\alpha_\kappa = P_\kappa Q_\kappa^{-1} , \quad \kappa = 1, 2, \ldots$$

where $P_{-1} = 1$, $P_0 = 2n + 1$, $Q_{-1} = 0$, and $Q_0 = 1$. Calculation by the FR algorithm is terminated when the modula of the increments of real and imaginary parts of the complex number α_κ do not exceed the preassigned small parameter $\varepsilon > 0$ in going to $\alpha_{\kappa+1}$

$$|\mathrm{Re}\,(\alpha_\kappa - \alpha_{\kappa+1})| < \varepsilon |\mathrm{Re}\,(\alpha_{\kappa+1})| , \tag{4.3}$$

$$|\mathrm{Im}\,(\alpha_\kappa - \alpha_{\kappa+1})| < \varepsilon |\mathrm{Im}\,(\alpha_{\kappa+1})| . \tag{4.4}$$

However, there is one more reason for termination of calculations by Eq. (4.2), namely, exponent overflow in the calculation of P_κ before conditions (4.3) and (4.4) are fulfilled. To pursue calculation of $\alpha(z)$, it is advisable to use the BR algorithm which in the case of Eq. (2.15) has the following form:

$$G_{\kappa+1}^j = 0, \; b_\kappa = 2n + 2\kappa + 1,$$

$$G_\kappa^j = -z^2 (b_\kappa + G_{\kappa+1}^j)^{-1} , \quad \kappa = n, n-1, \ldots, 1 , \tag{4.5}$$

$$\alpha_j = b_0 + G_1^j .$$

Calculation by Eq. (4.5) is repeated for $j = m + 1, m + 2, \ldots$, until conditions (4.3) and (4.4) will be fulfilled. A disadvantage of the BR algorithm is impossibility to use any intermediate term of the sequence in further calculations. Note that the use of the quadruple–precision numbers in the summation of continued fraction (2.15) does not provide any benefit until ε starts to increase the length of the real number. Therefore, for $\varepsilon \ge 10^{-6}$ it seems to be reasonable to

perform the summation of the single–precision numbers in Eq. (2.15). This combined sequence of the $\alpha(z)$ calculations proposed by us ensures a possibility of using earlier calculated terms in further calculations (as part of the FR algorithm) and eliminates the exponent overflow in calculating the intermediate quantities in going to the BR algorithm. At the same time, this method is capable of minimizing the effect of disadvantages peculiar to each of these algorithms and making the calculations of α many times faster, especially for large values of $|z|$ and small values of n and ε. At the same time for small ratios $n|z|^{-1}$ the calculations of $\alpha(z)$ even by the proposed combined method require the large number of iterations. Thus a decrease of the random–access memory capacity is accompanied by a significant increase in execution time for $n|z|^{-1} \ll 1$.

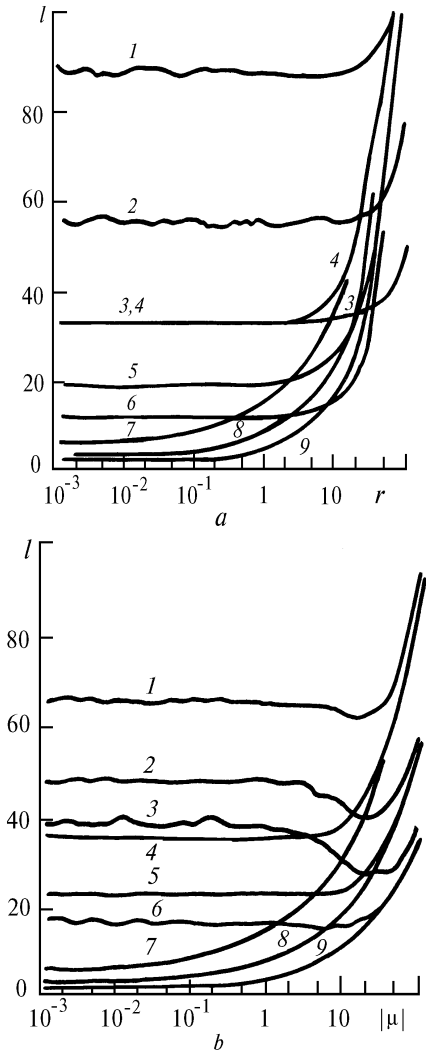

FIG. 2 Lengths l_1, l_2, and l_3 of the sequences of the logarithmic RBF1 derivatives correctly calculated for the single–precision (curves 3, 6, and 9), double–precision (curves 2, 5, and 8), and quadruple–precision complex numbers (curves 1, 4, and 7). The real part r of the argument (a) and the modulus of the negative quantity μ *(b) are plotted along the x axis. a) Curves1–3 are for* $\mu = -100$, *curves 4–6 are for* $\mu = -10$, *and curves 7–9 are for* $\mu = -10^{-2}$; *b) curves1–3 are for* $r = 30$, *curves 4–6 are for* $r = 10$, *and curves 7–9 are for* $r = 10^{-2}$.

Figure 1 shows the results of calculation of $\mathrm{Re}\{A_n\}$ (curve *1*) and $\mathrm{Im}\{A_n\}$ (curve *2*) by continued fraction (4.1). One can see that curves *1* and *2* are in a good agreement with A_n calculated by forward recursion (1.3). Moreover, for $n|z|^{-1} \gg 1$ curves *1* and *2* tend to asymptotic values of $\mathrm{Re}\{A_n\}$ and $\mathrm{Im}\{A_n\}$ calculated by Eq. (1.3) and shown by straight line *9* in Fig. 1.

5. CONCLUSION

In calculating the sequence of the logarithmic derivative $A_n(z)$ by backward recursion (1.1) it is better to use the asymptotic value obtained from Eq. (1.3) instead of Eq. (1.2) as an initial one. To reduce the random–access memory capacity, it is advisable to calculate by forward recursion (3.1)–(3.3) instead of backward one. Accumulated errors creeping in calculations of the quadruple–precision numbers by Eqs. (3.1)–(3.3) become pronounced only after the summation of the Mie series terminates.

Correctness of calculated values of the logarithmic derivative should be estimated by Eqs. (2.11)–(2.14). Calculations for the quadruple–precision numbers significantly increase the execution time. In addition, they are not implemented in translators preceding FORTRAN–77. Calculation of the correct sequence A_n for the single–precision numbers is ensured by the combined algorithm according to which forward recursion (3.1)–(3.3) is employed for $n < 0.3|z| + 1$, while for $n \geq 0.3|z| + 1$ A_n is determined from continued fraction (4.1)–(4.5). Formulas (4.1)–(4.5) can be used for calculation of any A_n, but the summation of continued fraction (2.15) requires more and more iterations as $n|z|^{-1}$ decreases. At the same time, for small $n|z|^{-1}$ the forward recursion ensures a necessary accuracy in calculating A_n. The combined FR–BR algorithm is best suited for calculation of continued fraction (2.15). In this case the calculation of Eq. (2.15) should be started from Eq. (4.2) at each step checking the fulfilment of conditions (4.3) and (4.4) and the case in which the modulus $|P_\kappa|$ is in excess of 10^{70}. If the absolute value $|P_m| > 10^{70}$ at the mth step, the calculations of the continued fraction are pursued at the $(m + 1)$th step by BR algorithm (4.5). Fulfilment of conditions (4.3) and (4.4) is indicative of the fact that the prescribed accuracy of calculations of the continued fraction is reached.

The technique developed in this paper removes all the limitations imposed on calculations of logarithmic derivatives of the Riccati–Bessel spherical functions of the complex argument and ensures the possibility of calculations by the Mie theory for arbitrary parameters of diffraction of particles and coefficients of light absorption by particles even when the random–access memory capacity is not more than 50 Kbytes.

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