CALCULATION OF THE RICCATI–BESSEL FUNCTIONS BY THE ASCENDING RECURSION

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Criteria for estimating the length of correctly calculated sequences of Riccati–Bessel functions of the first kind (RBF1) are constructed. The dimensions of sequences correctly calculated by the ascending recursion using single, double and fourfold precision of the representation of the complex numbersare studied. Algorithms of the precision control of the RBF1 calculations are proposed that, provide numerical studies based on the Mie theory to be done without operational storage redundancy for the RBF1 arrays that, in turn, facilitates on the Mie theory calculations up to extremely great values of the diffraction parameter of aerosol particles (~ 10^6 and more).

Explosion of aerosol particles under the effect of a strong light beam, as well as tension in solid particles, and formation micro squares of plasma inside a particle are studied based on numerical simulations of the radiation intensity distribution inside a particle using the Mie theory.[1] Terms of the Mie series are functionals which include the Riccati–Bessel functions of the first kind (RBF1) $\varphi_k(z)$. Calculations of the RBF1 of complex argument come across specific difficulties.[2,3] For this reason there are no standard programs for calculating the RBF1 of complex argument. An increase of the RBF1 calculation potentialities due to transition from the single precision of calculations to the double one is analyzed in Ref. 4. This paper analyzes a possibility of using the ascending recursion of the type described in Refs. 5–7

$$f_{l+1}(z) = \frac{2l+1}{z} f_l(z) - f_{l-1}(z) , \qquad (1)$$

which is valid for all Riccati–Bessel functions. It is accumed here that according to Refs. 5 and 7 first two functions $\varphi_0(z)$ and $\varphi_1(z)$ are equal to

$$\varphi_0(z) = \sin z, \qquad (2)$$

$$\varphi_1(z) = \frac{\sin z}{z} - \cos z . \qquad (3)$$

Errors of calculation by formula (1) are due to accumulation of the $\varphi_l(z)$ calculation inaccuracy with growth of l. Figure 1 presents the results of calculations of real (Fig. 1*a*) and imaginary (Fig. 1*b*) parts of sequences of the Riccati–Bessel functions of the first kind of the complex argument $z = 10 - i10$ performed by the ascending recursion (1) with single (curve *1*), double (curve *2*), and fourfold (curve *3*) precision. The abscissa of this graph is the subindex of the functions. Figure 1 shows that at initial steps the results of calculations by the ascending recursion calculation is dependent of the precision of a complex number representation. However, starting with the number l_1 the calculation with single precision leads to the exponential growth of error. At the same time the double–precision calculations do not lead to noticeable errors at a greater k values up to k equal to l_2 which exceeds the value l_1.

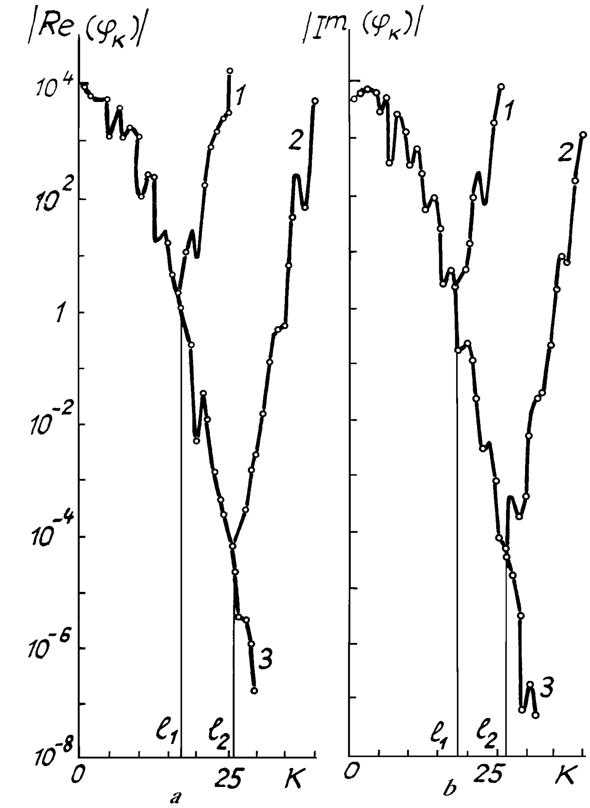

FIG. 1. Absolute value of real (Fig. 1a) and imaginary (Fig. 1b) parts of the sequences of the Riccati–Bessel function of the first kind of a complex argument $10 - i10$*, which are calculated by formula (1) with single (curve 1), double (curve 2), and fourfold (curve 3) precision. The abscissa of this graph is the subindex of the RBF1.*

The numbers l_1 and l_2 characterizing the dimensions of the RBF1 sequences which can be calculated with acceptable accuracy using the single– and double–precision representation of a complex number are determined by the values of real r and imaginary μ parts of the complex argument $z = r + i\mu$. Signs of r and μ do not influence on the

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size of the RBF1 sequences l_1 and l_2. For example, $l_1 = 14$ and $l_2 = 25$ for all complex arguments like $z_1 = 10 + i10$, $z_2 = 10 - i10$, $z_3 = -10 + i10$, and $z_4 = -10 - i10$. Similarly, if $|r| = 1$ and $|\mu| = 10$, then independently of signs of r and μ, l_1 is equal to 8 and $l_2 = 16$.

Figure 2*a* presents the dependences of l_1 (curves *1*, *3*, and *5*–*7*) and l_2 (curves *2*, *4*, *6*, *8*, and *9*) on the value of the real part $|r|$ of argument with a fixed value of the imaginary part $|\mu| = 10^{-2}$ (curves *1* and *2*), 30 (curves *3* and *4*), 50 (curves *5* and *6*), 100 (curves *7* and *8*), and 160 (curves *6* and *9*). Figure 2*b* presents the dependences of l_1 (curves *1*, *3*, *5*, and *7*) and l_2 (curves *2*, *4*, *6*, and *8*) on $|\mu|$ at a fixed value of the real part $|r| = 10^{-2}$ (curves *1* and *2*), 1 (curves *3* and *4*), 30 (curves *5* and *6*), and 50 (curves *7* and *8*).

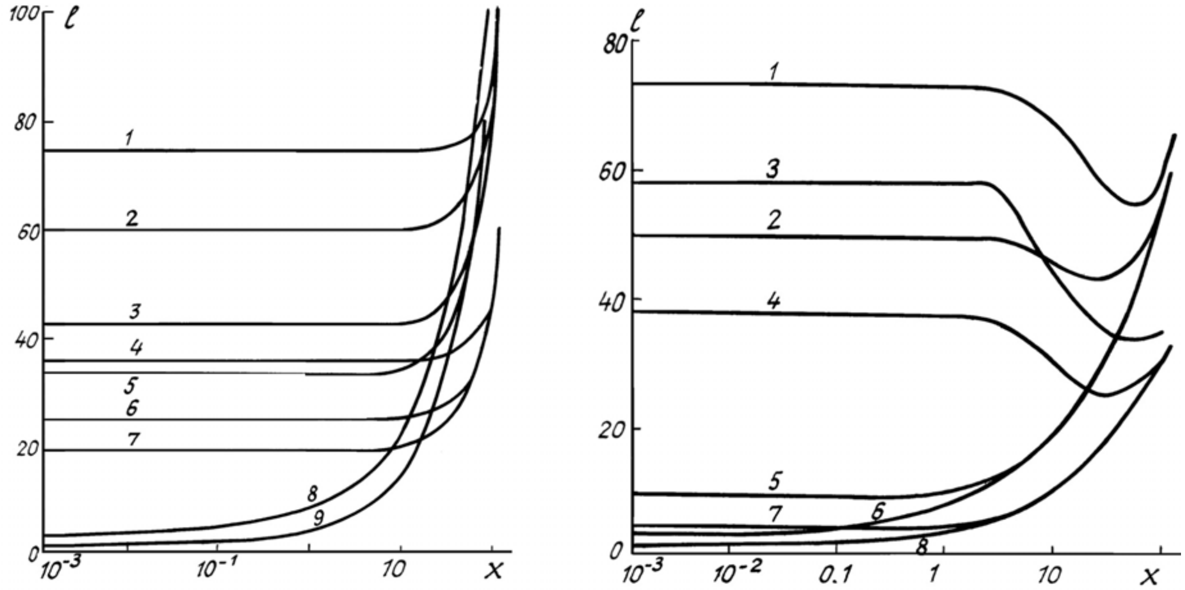

FIG. 2. The dimensions l_1 and l_2 of the RBF1 sequences correctly calculated using single– and double–precision representation of complex numbers.

In Fig. 2a the abscissa is the absolute value of the real part $|r|$ of the argument; the absolute value of the imaginary part $|\mu|$ is 10^{-2} (curves *1* and *2*), 30 (curves *3* and 4), 50 (curves *5* and *6*), 100 (curves *7* and *8*), and 160 (curves *6* and *9*). The first curve number in patentheses denote the curve corresponds to l_1 and the second one to l_2. In Fig. 2*b* the abscissa is the absolute value $|\mu|$; the value $|r| = 10^{-2}$ (curves *1* and *2*), 1 (curves *3* and *4*), 30 (curves *5* and *6*), 50 (curves *7* and *8*).

Let us denote the varying value of the argument (in the case of Fig. 2*a* it is $|l|$ and for Fig. 2*b* $|\mu|$), by x and the value of a parameter (for Fig. 2*a* it is $|\mu|$, and for Fig. 2*b* $|r|$) by p. Figures 2*a* and *b* show that for $x \le p$ the values l_1 and l_2 are in dependent of x and are determined by the value p

$$l_1 \approx c_1 |p| + 1 \,, \tag{4}$$

$$l_2 \approx c_2 |p| + 3 \,, \tag{5}$$

where $c_1 \approx 0.5$–0.8, and $c_2 \approx 1$. An exception is made for the region of the minima in $l_1(z)$ and $l_2(z)$ at $|\mu| \ge 10$ (Fig. 2*b*). For $x > p$ the values l_1 and l_2 cease to depend on the parameter value. As can be seen from Figs. 2*a* and *b* all curves l_1 and l_2 tend to confluence into two groups. The ascending recursion method makes it possible to calculate the RBF1 for $|r| \le \pi \cdot 2^{18}$ and $|\mu| \le 8.08$ (single precision), $|r| \le \pi \cdot 2^{50}$ and $|\mu| \le 17.3$ (double precision), and $|r| \le \pi \cdot 2^{100}$ and $|\mu| \le 37.4$ (fourfold precision). There are two restrictions imposed on $|r|$: first an acceptable value of arguments of the sine and cosine, functions and, second, a restriction typical of calculating exponential function. In many cases the value l_1 is insufficient for making calculations based on the Mie theory, alternatively, the value l_2 is quite sufficient for this purpose. However, it is reasonable to foresee the possibility of using the RBF1 sequence whose dimension essentially exceeds l_2. Such a possibility is given by the RBF1 calculations by formula (1) with the fourfold precision. Actually, since the transition from the single to double precision has yielded nearly twofold increase of the dimension of the correctly calculated sequence (Fig. 1), the transition to the fourfold precision may lead to further increase of the dimension. And then the problem arises on determination of the dimension of the RBF1 sequence correctly calculated by formula (1) using the fourfold precision of a complex number representation. If further increasing the precision of a complex number representation (for example, transition to the eightfold precision) is impossible, for testing the precision of the RBF1 calculations it is expedient to make use of the vanishing behavior of the following functions with increasing l

$$F_1(l) = \sum_{\kappa=0}^{l} (2\kappa + 1) \left(\frac{\varphi_\kappa(z)}{z}\right)^2 - 1 \,; \tag{6}$$

$$F_2(l) = \sum_{\kappa=0}^{l} (-1)^\kappa (2\kappa + 1) \frac{2\varphi^2(z)}{z \sin(2z)} - 1 \,; \tag{7}$$

$$F_3(l) = \xi_l(z)\,\varphi_l'(z) - \xi_l'(z)\,\varphi_l(z) - i\ ; \quad (8)$$

$$F_4(l) = \varphi_{l-1}(z)\,\eta_l(z) - \varphi_l(z)\,\eta_{l-1}(z) - 1\ ; \quad (9)$$

$$F_5(l) = \varphi_{l-1}(z)\,\eta_{l+1}(z) - \varphi_{l+1}(z)\,\eta_{l-1}(z) - \frac{2l+1}{z}\ ; \quad (10)$$

$$F_6(l) = \varphi_l(z) + i\eta_l(z) - \xi_l(z)\ , \quad (11)$$

where $\eta_l(z)$ and $\xi_l(z)$ are the Riccati–Bessel functions of the second and third kinds, $\varphi_l'(z)$ and $\xi_l'(z)$ are the RBF2 and RBF3 derivatives calculated by formulas from Refs. 5 and 7

$$f_l'(z) = f_{l-1}(z) - \frac{l}{z} f_l(z)\ .$$

The RBF2 and RBF3 calculations by formula (1) does not yield essential errors. Formulas for the first two functions $\eta_l(z)$ and $\xi_l(z)$ needed for calculations by formula (1) have the form[7]

$$\eta_0(z) = \cos z\ ;\ \ \eta_1(z) = \sin z + \frac{\cos z}{z}\ ;$$

$$\xi_0(z) = i\exp(-iz)\ ;\ \ \xi_1(z) = \left(\frac{i}{z} - 1\right)\exp(-iz)\ .$$

Relations (6) and (7) are modifications of formulas for infinite RBF1 series[5]

$$\sum_{\kappa=0}^{\infty} (2\kappa+1)\left(\frac{\varphi_\kappa(z)}{z}\right)^2 = 1\ ;$$

$$\sum_{\kappa=0}^{\infty} (-1)^\kappa (2\kappa+1)\frac{\varphi_\kappa^2(z)}{z} = \frac{\sin 2z}{2}$$

convenient for testing the series convergency. Formulas (8)–(11) are derived using algebraic transformations of known properties of the RBF. At $|\mu| < 1$ all criteria (6)–(10) show sharp increase of the functions $F_1(l)$, $F_2(l)$, ..., $F_5(l)$ starting from close l, the least of them can be taken as the RBF1 sequence dimension l_4, wich is correctly calculated by formula (1). Formula (11) is convenient for estimating l_4 only at small $|\mu| \le 10^{-4}$. The validity of relations (8)–(11) is worsened with increase of $|\mu|$. For example, at $|\mu| = 50$ these formulas are absolutely inapplicable to estimation of l_4. Calculations made by formulas (6) and (7) in a wide range of $|\mu|$ values (from 10^{-3} up to 50) show that minima in the dependences $F_1(l)$ and $F_2(l)$ always correspond to close l values, the least of them providing a reliable estimation of l_4. It should be noted that at small $l < l_2$ dependences $F_1(l)$ and $F_2(l)$ may have pulsations. So the search for $F_1(l)$ and $F_2(l)$ minima is advisable to be done starting with $l_1 > l_2$. The present study opens wide perspectives for calculations based on the Mie theory. Without using any intermediate data sets one can perform the RBF1 calculations up to large values of the argument ($4\cdot10^5 - i100$) by formula (1). The counter recursion should demand too great operational memory for storing intermediate data, which should be corrected at the final stage of calculations.

Using the above–mentioned method the calculations of cross sections of attenuation and scattering of light by a particle with a diffraction parameter of 10^6 and a refractive index of $1.33 - i10^{-6}$ takes only few hours of ES–1046 computer time and needs a few tens of kilobytes of operational memory. Thus, the method eliminates the limitations on a particle size and allows a wide use of the PCs for making calculations based on the Mie theory. The calculations for extremely large diffraction parameters that earlier required big machines now can be performed on any computer if only it has sufficient word length for a relevant representation of a complex number.

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