

Study of methods and errors in computation of Ricatti–Bessel functions

N.P. Romanov

RPA “Typhoon”, Obninsk, Kaluga Region

Received April 20, 2007

The dependence of the Ricatti–Bessel (RB) function of the 1st (RB1), 2nd (RB2), 3rd (RB3), and 4th (RB4) kinds of the real x and complex $z = x + iy$ arguments on their order ℓ are studied analytically and numerically. The domains of RB function's module increase with increase of ℓ , tolerant to the forward-recurrence errors, and of module decrease, tolerant to the backward-recurrence one, are found out. The domain of stability of the forward recurrence for RB1 function at $x \gg 1$ is determined by the relation $0 \leq \ell \leq \ell_{\max} = x - 0.5 - 0.80861x^{1/3} - 0.1635x^{-1/3}$ on condition that $|y| \leq 0.4 \log x + 0.5$; here the fractional error of the forward recurrence increases with an increase of ℓ proportionally to $\ell^{1/2}$. If $\ell > \ell_{\max}$, the forward recurrence results in generation of the function equal to the sum of RB1 and RB2 functions instead of the function RB1. The fractional error of the backward recurrence for the RB1 function is virtually independent of ℓ in the whole ℓ range, increases by the $|z|^{1/2}$ law with an increase of z modulus, and is comparable with the forward-recurrence error at $\ell = \ell_{\max}$ under the above limitations on y . To obtain the initial RB1 values in the backward recurrence, a simplified calculation procedure for the ratio of these functions of the neighboring orders with the use of a continued fraction is suggested, an additional forward-recurrence computation of the RB2 function at $y = 0$ or RB3 at $y > 0$, and the use of the Wronskian of the corresponding functions. A FORTRAN program for computing the above-mentioned ratio of RB1 functions is presented. In the domains of stability, the main computation error of functions of decimal arguments can be determined by the error of their conversion into the binary computer system.

Introduction

Computation of parameters of electromagnetic radiation interaction with spherical particles is the grounds for atmospheric optics and is reduced to the summation of Mie series.^{1–3} Radial coefficients of these series are expressed in terms of Ricatti–Bessel functions of the first $\psi_\ell(z)$ (RB1) and second $\chi_\ell(z)$ (RB2) kinds. Based on the performed investigations, a common computing recommendation is the use of forward recurrence for RB2 and backward recurrence for RB1 functions.^{3–9} However, we don't know works with analytical proof of this statement, the lack of which casts some doubts on the accuracy of computation results. Thus, the double-precision forward recurrence is used in Ref. 3 for RB1 function of the real argument, which, in the authors' opinion, does not insure against large computation errors in the uncontrollable region $\ell \gg x$. The authors specially warned against computing the function $\psi_\ell(z)$ in unstudied regions $\ell - z$.

In this work, the errors of RB function recursive computation are estimated and the domains of stability of recurrence procedures are deduced. These domains are determined from the analysis of RB function properties. A technique for simultaneous computation of RB1 and RB2 functions is suggested. To initialize the backward recurrence, a simplified continued-fractions scheme is worked out for computing the ratio of RB1 functions of neighboring orders and the use of the Wronskian for generating the functions. The newly suggested algorithms are

numerically tested. The text of a FORTRAN subroutine for the RB1 function ratio computation is given in the Appendix.

1. Basic relationships

In the Mie theory,^{1–3} the RB functions of the first $\psi_\ell(z)$ and second $\chi_\ell(z)$ kinds are used, which are two independent solutions of the differential equation⁴

$$\Phi_\ell''(z) - \left(\frac{\ell(\ell+1)}{z^2} - 1 \right) \Phi_\ell(z) = 0 \quad (1)$$

defined by the series of the form

$$\psi_\ell(z) = \frac{z^{\ell+1}}{(2\ell+1)!!} \times \left[1 - \frac{z^2/2}{1!(2\ell+3)} + \frac{(z^2/2)^2}{2!(2\ell+3)(2\ell+5)} - \dots \right]; \quad (2)$$

$$\chi_\ell(z) = \frac{(2\ell-1)!!}{z^\ell} \times \left[1 + \frac{z^2/2}{1!(2\ell-1)} + \frac{(z^2/2)^2}{2!(2\ell-1)(2\ell-3)} + \dots \right]. \quad (3)$$

Another pair of independent solutions is the functions $\eta_\ell(z)$ (RB3) and $\zeta_\ell(z)$ (RB4) defined by the equations

$$\eta_\ell(z) = \psi_\ell(z) - i\chi_\ell(z); \quad (4)$$

$$\zeta_\ell(z) = \psi_\ell(z) + i\chi_\ell(z). \quad (5)$$

Recurrence relations between functions of different orders have the form

$$\Phi_{\ell+1}(z) = \frac{2\ell+1}{z}\Phi_\ell(z) - \Phi_{\ell-1}(z), \quad (6)$$

$$\Phi'_\ell(z) = \Phi_{\ell-1}(z) - \frac{\ell}{z}\Phi_\ell(z). \quad (7)$$

The Wronskian of two independent functions $\psi_\ell(z)$ and $\chi_\ell(z)$ is

$$\begin{aligned} W(\psi, \chi) &= [\psi'_\ell(z)\chi_\ell(z) - \psi_\ell(z)\chi'_\ell(z)] = \\ &= [\psi_{\ell-1}(z)\chi_\ell(z) - \psi_\ell(z)\chi_{\ell-1}(z)] = 1. \end{aligned} \quad (8)$$

For further use the Wronskian expressions of the following pairs of functions are helpful:

$$W(\psi, \eta) = [\psi_{\ell-1}(z)\eta_\ell(z) - \psi_\ell(z)\eta_{\ell-1}(z)] = -i, \quad (8a)$$

$$W(\psi, \zeta) = [\psi_{\ell-1}(z)\zeta_\ell(z) - \psi_\ell(z)\zeta_{\ell-1}(z)] = i. \quad (8b)$$

RB functions at integer ℓ are expressed in terms of trigonometric functions, in particular:

$$\begin{aligned} \psi_0(z) &= -\chi_{-1}(z) = \sin(z), \\ \psi_{-1}(z) &= -\chi_0(z) = \cos(z), \\ \eta_{-1}(z) &= i\eta_0(z) = \exp(iz), \\ \zeta_{-1}(z) &= -i\zeta_0(z) = \exp(-iz). \end{aligned} \quad (9)$$

Equations (9) along with Eq. (6) allow the forward recurrence generation for computing RB functions for integer $\ell \geq 1$, used in the Mie series. Equations (6) are used for the backward recurrence generation as well, but the choice of initial values in this case is more complicated. The review and realization of different schemes of the backward recurrence generation are given in Refs. 5–10. The ratio of functions of two neighboring orders $R_\ell^q(z) = \Phi_{\ell-1}(z)/\Phi_\ell(z)$ is of great importance here; the forward and backward recurrence relations for this ratio follow directly from Eq. (6)

$$R_{\ell+1}(z) = \left[\frac{2\ell+1}{z} - R_\ell(z) \right]^{-1}, \quad (10a)$$

$$R_\ell(z) = \frac{2\ell+1}{z} - \frac{1}{R_{\ell+1}(z)}. \quad (10b)$$

2. Estimation of the errors of recurrence procedures

To estimate the errors in computation of RB functions, consider the ratio of $R_\ell(z)$ functions, since it depends only on single magnitude of a neighboring order while the functions themselves depend on two functions of two neighboring orders. In this case, analytical relationships for the recurrent process

errors can be obtained. Introduce the fractional error g_ℓ of calculation of the ratio of $R_\ell(z)$; in this case the computed value $\tilde{R}_\ell(z)$ is represented in the form

$$\tilde{R}_\ell = R_\ell(1 + g_\ell). \quad (11)$$

Substituting Eq. (11) in Eq. (10b) and neglecting the error of $(2\ell+1)/z$ computation, we obtain

$$g_{\ell+1}(1 + g_{\ell+1})^{-1} = R_\ell R_{\ell+1} g_\ell,$$

assuming $|g_{\ell+1}| \ll 1$, obtain

$$g_{\ell+1} = g_\ell R_\ell R_{\ell+1} \equiv g_\ell \frac{\Phi_{\ell-1}}{\Phi_{\ell+1}}. \quad (12)$$

A similar relation was obtained in Ref. 8 and used to validate the necessity of backward recurrence for $R_\ell^y(z)$ at complex z . Applying Eq. (12) k times and carrying out necessary cancellations, we obtain

$$g_{\ell+k} = g_\ell \frac{\Phi_\ell \Phi_{\ell-1}}{\Phi_{\ell+k} \Phi_{\ell+k-1}}, \quad g_{\ell+1} \dots g_\ell \ll 1. \quad (13)$$

Equations (12) and (13) are valid for estimating errors of both forward and backward recurrences. Note that these equations are not accurate, because errors of addition, division, and multiplication operations due to data storage limitation have not been taken into account when computing the equations. However, they allow a qualitative conclusion that the forward recurrence error should be damped in the domain of function module increase with ℓ increase. It can be said that this reflects more general conclusion that any difference forward-applied equation is effective merely for computing “the largest” solution of this equation.⁷ Naturally, the domain of stability of the backward process is within the domain of function module decrease as ℓ increases.

It follows from the above that to chose the computation method, to chose a computation method it is necessary to know the qualitative dependence of FB functions on ℓ in different ranges of complex z . Since the dependences of RB functions of real argument are simpler, first consider this case.

3. Properties of RB functions of real argument

The character of the dependences of RB functions on x at fixed ℓ and on ℓ at fixed x is described analytically and graphically in Ref. 4 and summarized below. At fixed ℓ and x increasing from 0 to the infinity, $\psi_\ell(x)$ first increases from infinitesimal quantities, defined by the first term of series (2), to the values greater than unit in the first maximum, determined by the first zero of the first derivative $\psi'_{\ell,1}$, then passes through the first zero of $\psi_{\ell,1}$, and again oscillates near the x axis approaching the harmonic x -dependence with the amplitude

tending to unit. Asymptotic decomposition of $\psi_{\ell,s}$ zeros for large ℓ is given in Ref. 4, and for $\psi'_{\ell,s}$ was obtained by the author in Ref. 11. At large ℓ , $\psi_{\ell}(x)$ in the first maximum approximately equals to⁴

$$\psi_{\ell}(\psi'_{\ell,1}) \approx 0.8458 \left(\ell + \frac{1}{2} \right)^{1/6}. \quad (14)$$

While x is rising from 0 to the infinity, $\chi_{\ell}(x)$ first decreases from the infinitely large quantities, defined by the first term of series (3), to the first zero of $\chi_{\ell,1}$, passes through the first maximum of the absolute value, determined by the first zero of the derivative $\chi'_{\ell,1}$, and again oscillates near the x axis with the amplitude converging to unit and the phase π -shifted relative to the phase of $\psi_{\ell}(x)$. The value of $\chi_{\ell}(x)$ in the first maximum of the absolute value at large ℓ is described by a similar dependence

$$\chi_{\ell}(\chi'_{\ell,1}) \approx -0.7184 \left(\ell + \frac{1}{2} \right)^{1/6}. \quad (15)$$

While x is rising from 0 to the infinity, the modules of $\eta_{\ell}(x)$ and $\zeta_{\ell}(x)$ decrease monotonically from the values, defined by the first term of series (3), to unit.

With fixed x and rising ℓ , $\psi_{\ell}(x)$, being in this case a continuous variable, oscillates with an increasing amplitude, attains its maximum at the point $\ell = \ell_{\max}^{\psi} = \ell_1^{\psi}$, determined by the relation $\psi'_{\ell,s}(x) = 0$, and again tends to zero like the first term of a series (2). Computational investigation of the dependence $\ell_{\max}^{\psi}(x)$ on the base of the dependence $\psi'_{\ell,s}$ [Ref. 11] results in the equation

$$\begin{aligned} \ell_{\max}^{\psi}(x) &= x - \frac{1}{2} - 0.808616x^{1/3} - 0.1635x^{-1/3}, \\ x \geq \psi'_{\ell,1} &\approx 2.74. \end{aligned} \quad (16)$$

The similar equation for the first zero of the function has the form

$$\begin{aligned} \ell_1^{\psi}(x) &= x - \frac{1}{2} - 1.855757x^{1/3} + 0.1146x^{-1/3}, \\ x \geq \psi_{\ell,1} &\approx 4.49. \end{aligned} \quad (17)$$

For further study, it is useful to know also the dependence $\ell_1^{\chi}(x)$, defined similarly. The following equation is obtained from the numerical analysis:

$$\begin{aligned} \ell_1^{\chi}(x) &= x - \frac{1}{2} - 0.931577x^{1/3} + 0.0256x^{-1/3}, \\ x \geq \chi_{\ell,1} &\approx 2.80. \end{aligned} \quad (18)$$

Similar procedure for $\ell_{\max}^{\chi} = \ell_1^{\chi}(x)$ results in the equation

$$\begin{aligned} \ell_{\max}^{\chi}(x) &= x - \frac{1}{2} - 1.821090x^{1/3} + 0.03045x^{-1/3}, \\ x \geq \chi'_{\ell,1} &\approx 4.48. \end{aligned} \quad (19)$$

According to the stated above, the following computation scheme for $\psi_{\ell}(x)$ of real argument, optimal in view of minimum errors, is emerged: forward recurrence is used for $\ell \leq \ell_{\max}^{\psi}$ and backward one – for $\ell > \ell_{\max}^{\psi}$. The question on domains separation for the complex z requires an individual study. Now consider the technique for computing $\psi_{\ell}(x)$ for arbitrary correlations between x and ℓ .

4. Technique for computing RB functions of real argument

Initial values of functions for backward recurrence were found out as follows. $R_{\ell}^{\psi}(x)$ are computed using continued fractions by the method¹² simplified as compared to the Lentz one in the way, described below; $\chi_{\ell-1}(x)$ and $\chi_{\ell}(x)$ for boundary values $\ell = \ell_b > \ell_{\max}^{\psi}$ are computed by the forward-recurrence method. Then $\psi_{\ell}(x)$ is computed with Wronskian (6) by the equation

$$\psi_{\ell}(x) = \frac{1}{R_{\ell}^{\psi}(x)\chi_{\ell}(x) - \chi_{\ell-1}(x)}, \quad (20)$$

and $\psi_{\ell-1}(x) = \psi_{\ell}(x)R_{\ell}^{\psi}(x)$ by definition. Note, that Equation (20) is free of errors when generating small value $\psi_{\ell}(x)$ at $\ell = \ell_b$, because it is generated from the division of unit by a larger value.

Errors of this scheme were computationally investigated using IBM PC with 24-bit floating-point representation. The main method was the comparison of single- and double-precision computations of the functions; FORTRAN language was used for the program.

It was estimated at the first stage of comparative computations, how computation errors depend on whether the fractional part of the decimal argument x can be finally expressed in the binary system, used in computers. Note, that all integers are convertible to the binary system. At the same time, the number's fractional part equal, e.g., to $0.1N$ ($N \neq 5, 10\dots$), can be represented only in the form of recurrent dyadic fraction.¹³ The error of a number conversion from one system notation to another is called system-notation error. Maximal relative value of the error for the binary system is

$$\max \left| \frac{\Delta x}{x} \right|_{10-2} = 2^{-q}, \quad (21)$$

where q is the number of bits using for mantissa. In our case, decimal $\max |\Delta x/x|_{10-2} = 6 \cdot 10^{-8}$. According to the investigations, the errors of single-precision computations of all RB functions in the domain of recurrence stability (in case of non-representability of the argument in the binary system) are finally caused by the system-notation error and are defined by the equation

$$\Delta \Phi = \Phi' \Delta x_{10-2}. \quad (22)$$

If the fractional part of x is binary representable, the only operation errors¹³ finally manifest themselves,

the study of which is the aim of this work. We realized this case by setting the fractional part of x as $1/2^n$, where n is integer. An absolute error of computing the basic functions $\sin x$ and $\cos x$ in this case has no trends with x increase and does not exceed $3 \cdot 10^{-8}$ in the studied range $x \leq 10^4$ at a single precision.

At the second stage, the dependence of the error on the hierarchy of operations in Eq. (4) was examined. It is turned out that the computation result differs only in case when the value $1/x$ is generated before the beginning of a recurrence process and then serves as a multiplier. This variant requires 1.5-fold shorter time, because the division is the most time-consuming operation and in this case it is carried out only once before the recurrence cycle. In all other cases computation time and result in Eq. (4) are the same; computation errors are usually less than in the case of $1/x$ generating. Hence, the study of errors of RB functions computation was mainly carried out with the operation hierarchy corresponding to Eq. (4).

General regularities of the error in the $\psi_\ell(x)$ and $\chi_\ell(x)$ forward-recurrence comparative calculations for $\ell \leq \ell_{\max}^{\psi}$ and $\ell \leq \ell_{\max}^{\chi}$, respectively, consist in the fact that with growing ℓ the absolute error oscillates with weakly increasing amplitude from the values, pointed above for $\sin x$ and $\cos x$, to those, defined for the both functions by one equation

$$|\Delta\psi_\ell(x), \Delta\chi_\ell(x)| \approx 2 \cdot 10^{-8} x^{2/3}, \quad \ell \approx \ell_{\max}^{\psi}, \quad \ell \approx \ell_{\max}^{\chi}. \quad (23)$$

At further ℓ increase, the absolute value of $\Delta\chi_\ell$ sharply increases, but the fractional error remains virtually constant and its average value is described by the equation

$$|\Delta\chi_\ell/\chi_\ell| \approx 2.5 \cdot 10^{-8} x^{1/2}, \quad \ell \geq \ell_1^{\chi}, \quad (24)$$

which well agrees with Eqs. (14), (15), and (23).

In the region $\ell > \ell_{\max}^{\psi}$, fractional and even absolute errors of $\psi_\ell(x)$ computation begin to rise quickly with rising ℓ . However, the value of Wronskian (8) remains equal to unit. This means that the computed value of $\tilde{\psi}_\ell(x)$ in this region is the sum

$$\tilde{\psi}_\ell(x) = \psi_\ell(x) + b\chi_\ell(x), \quad \ell > \ell_{\max}^{\psi}. \quad (25)$$

When x varies, both sign and value of b can change. The behavior of b for average values can be described by the following equation:

$$|b| \approx 2 \cdot 10^{-8} x^{1/2}. \quad (26)$$

Already at small ℓ exceeding over ℓ_{\max}^{ψ} , the second term in Eq. (25) is determinative, i.e., the forward-recurrence calculated $\tilde{\psi}_\ell(x)$ is virtually proportional to $\chi_\ell(x)$ and the obtained R_ℓ is $R_\ell^{\chi}(x)$. The obtained result, seemingly paradoxical, approves the above statement that any forward-applied difference equation is effective only in calculating the "greatest" solution of this equation.⁷ The increase of absolute [Eq. (23)] and fractional errors [which follows from the comparison of Eq. (23) with Eqs. (14)

and (15)] in the domain of stability can be explained by the fact that damping Equation (13) only partially damps the operation errors; as a result, the calculation error is proportional to the square root of the number of operations.

The absolute backward recurrence error was studied for ℓ_b , defined by the equation $\ell_b = x + 4x^{1/3} + 8$ which, according to Refs. 3 and 6, provides for proper summation of the Mie series; in this case, the fractional error of backward-recurrence calculation of $\psi_\ell(x)$ for the fixed x is virtually constant in the whole ℓ range. Its dependence on x is approximately described by equation

$$|\Delta\psi_\ell/\psi_\ell| \approx (3 \div 5) \cdot 10^{-8} x^{1/2}, \quad (27)$$

which is closely agrees with those for the functions $\psi_\ell(x)$ at $\ell = \ell_{\max}^{\psi}$ and $\chi_\ell(x)$ at $\ell \geq \ell_{\max}^{\chi}$ [see Eq. (24)] for the forward recurrence. The above statements are illustrated by Fig. 1, where absolute forward and backward recurrence errors for $\psi_\ell(x)$ are shown for $x = 1000$ (binary representable integer) and $x = 1000.1$ (the number, non-representable in the binary system); they are represented by the domains of their variability for $\ell < \ell_{\max}^{\psi}$.

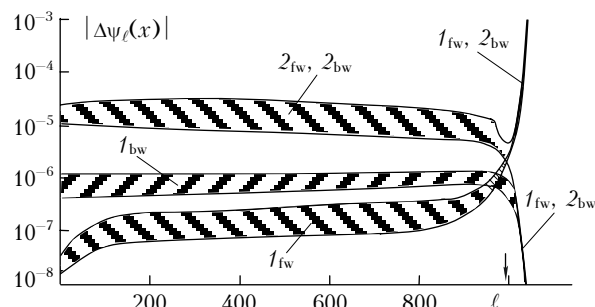


Fig. 1. Absolute errors of RB1 functions calculation for $x = 1000$ (curves 1) and $x = 1000.1$ (curves 2) by the forward (curves 1_{fw}, 2_{fw}) and backward (curves 1_{bw}, 2_{bw}) recurrence methods.

The position of $\ell = \ell_{\max}^{\psi}$ is pointed out by the arrow. As is well seen, in case of binary representable numbers the forward recurrence gives a better precision for $\ell < \ell_{\max}^{\psi}$, while the backward one – for $\ell > \ell_{\max}^{\psi}$; errors of both recurrence become equal near $\ell = \ell_{\max}^{\psi}$. At the same time, the error of number conversion almost equalizes the errors of both recurrences in the range $\ell < \ell_{\max}^{\psi}$, which exceed the computation error for the case, shown in Fig. 1, by more than an order of magnitude. Sharp increase of the error at $\ell > \ell_{\max}^{\psi}$ is caused by the recurrence process change to generation of a function proportional to $\chi_\ell(x)$.

5. Properties and errors of the technique for computing RB functions of complex argument z

When describing properties of RB function of complex argument, restrict ourselves by the region

$0 \leq \theta = \arg z \leq \pi/2$, since in other sectors RB functions are expressed through functions of this sector via complex conjugation or sign change. Thus, $\psi_\ell(z^*) = \psi_\ell^*(z)$ and $|\eta_\ell(z^*)| = |\zeta_\ell(z)|$. We use two equivalent complex-number notations $z = x + iy = r(\cos\theta + i\sin\theta)$. In the latter, r is the modulus and θ is the amplitude of complex number.

It follows from RB functions in the form of series (2) and (3), that the dependence of the functions modules on the argument modulus at $\ell \gg r$ should be similar to those for real argument. At the same time, as it follows from Eq. (9) for RB functions at $\ell = 0$, the modules of these functions at small ℓ have exponential dependence on y :

$$|\psi_0(z)| = |\chi_0(z)| = \exp(y)/2, \tag{28a}$$

$$|\eta_0(z)| = \exp(-y), \tag{28b}$$

$$|\zeta_0(z)| = \exp(y). \tag{28c}$$

The functional dependence at intermediate values of ℓ defies simple analysis and can be obtained from numerical computations. Examples of such computations for $x, y = 10$ are given in Ref. 14, where the domain of forward recurrence applicability is analyzed when using single, double, triple, and quadruple precision.

In this work, the computation results of ℓ -dependence of the RB1 function for $r = 10$ and several values of the amplitude, shown in Fig. 2, illustrate the function behavior at large values of its argument.

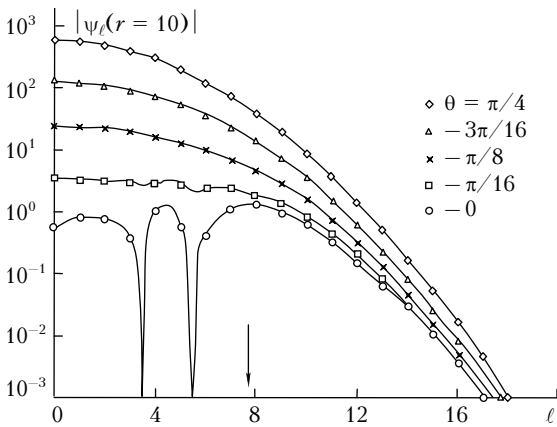


Fig. 2. Dependence of the RB1 function module on ℓ at $r = 10$ and different amplitudes θ .

The markers correspond to the calculated values at integer ℓ , while solid curves, connecting the marked points, represent RB1 values at intermediate ℓ . The arrow points to the ℓ value, at which RB1 attains its maximum at real argument, i.e., $\ell_{\max}^\psi(10 + i \cdot 0) = 7.68$. Sharp RB1 function decrease is observed with the order increase, which, according to the above consideration, rejects the forward recurrence applicability at large θ . The behaviors of RB1 and RB2 at large r and small θ is shown in Fig. 3 and those of RB3 and RB4 – in Fig. 4.

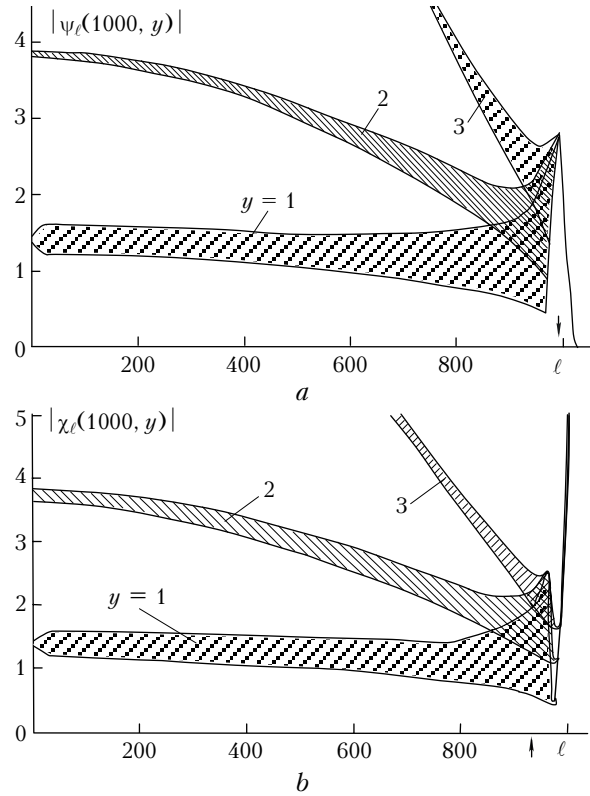


Fig. 3. Dependences of the modules of RB1 and RB2 functions on ℓ at fixed $x = 10^3$ and different y . The arrows correspond to the values of ℓ_{\max}^ψ and ℓ_{\max}^χ for $x = r$ according to Eqs. (16) and (19), respectively.

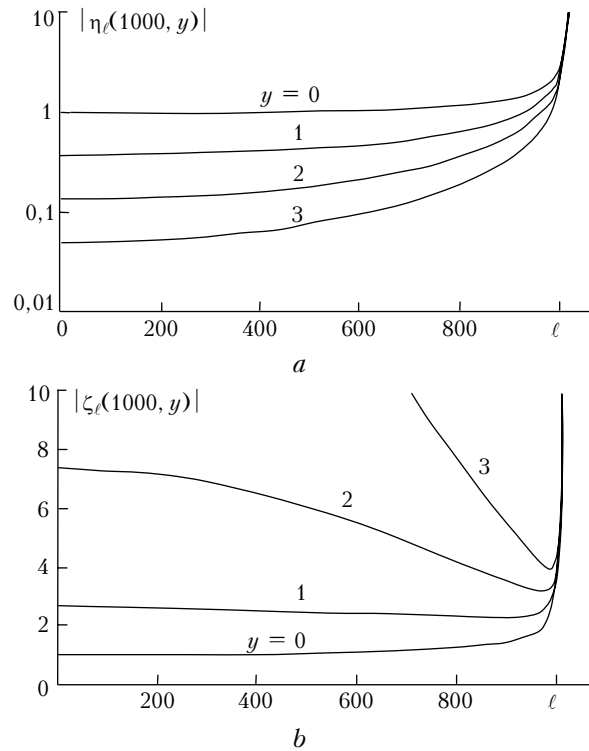


Fig. 4. Dependences of the modules of RB3 and RB4 functions on ℓ at fixed $x = 10^3$ and different y (the values are near the curves).

In view of oscillating character of RB1 and RB2, the shading in Fig. 3 points to the ranges of their modules. It is seen that the oscillation amplitudes of RB1 and RB2 decrease with the increase of the arguments, while their average values increase. The above-noted behavior of the functions at small [execution of Eq. (28)] and large (the same dependence at fixed r) values of ℓ is evident. In particular, the module maximum slightly changes at ℓ_{\max}^{ψ} and ℓ_{\max}^{χ} , defined by Eqs. (16) and (19), respectively, when changing x to r . Equaling Eqs. (28a) and (14), obtain the condition of equality of the RB1 module at points $\ell = 0$ and $\ell = \ell_{\max}^{\psi}$, which determines the limiting point of the forward recurrence stability at $\ell \leq \ell_{\max}^{\psi}$:

$$y \leq 0.41 \log x + 0.5. \tag{29}$$

There is a decrease of the function module for RB3 and an increase – for RB4 with an increase of the imaginary part of z . It is seen from Fig. 4b, that the RB4 module at $y > 0$ has the minimum near $\ell = x$, the depth of which increases with the increase of y . Hence, taking Eq. (13) into account, the conclusion can be drawn that the forward recurrence is unstable for this function. The RB3 module monotonically increases with an increase of ℓ for all $y \geq 0$ (see Fig. 4a), therefore, the forward recurrence for the function $\eta_{\ell}(z)$ at $0 \leq \arg z \leq \pi/2$ is to be stable.

Numerical check has shown that the behavior of the absolute value of forward-recurrence fractional error for this function weekly depends on θ and virtually repeats the regularities of errors' behavior of the RB2 function of real argument. Hence, to obtain $\psi_{\ell}(z)$ for large ℓ at the known $R_{\ell}^{\psi}(z)$, it is necessary to use Eq. (8a), which results in the following equation:

$$\psi_{\ell}(z) = \frac{-i}{R_{\ell}^{\psi}(z)\eta_{\ell}(z) - \eta_{\ell-1}(z)}. \tag{30}$$

The examples of errors of forward and backward [with the use of Eq. (30)] recurrences are shown in Fig. 5.

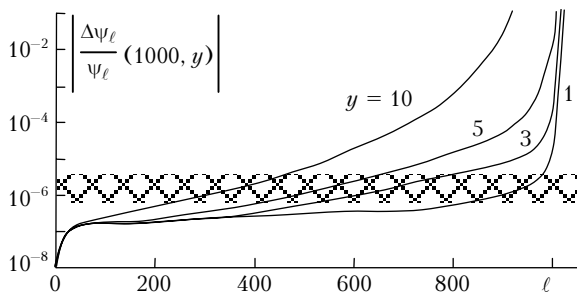


Fig. 5. Module of the fractional error of RB1 function computation as a function of ℓ at $x = 1000$ and different y for the forward (solid curves, numbers of which correspond to the values of y) and backward (shaded area) recurrences.

The numbers of curves for the forward recurrence correspond to the values of y . The errors

of backward recurrence for the same y are in the shaded horizontal area. The following regularities of the behavior of forward and backward recurrence errors, when computing RB1 functions of complex arguments, are revealed from Fig. 5 and computations for other values of z and ℓ : the backward recurrence error at fixed z is almost constant for all ℓ , weekly depends on θ , and is within the limits

$$\left| \frac{\Delta\psi_{\ell}(z)}{\psi_{\ell}(z)} \right| = (3 \div 6) \cdot 10^{-8} r^{1/2}; \quad 0 \leq \theta \leq \frac{\pi}{2}, \quad \ell \leq \ell_b. \tag{31}$$

This equation actually includes Eq. (27), obtained for real arguments. Under fulfillment of Eq. (29), the forward recurrence gives smaller error for $\ell < \ell_{\max}^{\psi}$ which equalizes with those for backward recurrence at $\ell = \ell_{\max}^{\psi}$. This boundary shifts to the left as y increases. Analytical relations for this case are not obtained in this work; this has been done in Ref. 14. At the end of this part note, that all conclusions about the stability of the recurrences for the RB1 functions directly relate to the functions ratio; the procedure for which is described below.

6. The choice and grounds for the algorithm of computing the RB1 functions ratio

To find the initial values $\psi_{\ell-1}(z)$ and $\psi_{\ell}(z)$ or their ratio, series (2) can be correctly used only under condition

$$2\ell > |z|^2, \tag{32}$$

when its terms decrease in absolute magnitude. At a smaller ℓ , the series' terms first increase in absolute magnitude up to values much greater than unit, therefore the value of sum in square brackets in Eq. (2) is determined by the difference of values much greater than the difference itself. The Taylor series' terms for the ratio can be obtained by division of the series for $\psi_{\ell-1}(z)$ and $\psi_{\ell}(z)$ and have the form

$$R_{\ell}^{\psi}(z) = \frac{2\ell + 1}{z} \times \left[1 - \frac{z^2}{(2\ell + 1)(2\ell + 3)} - \frac{z^4}{(2\ell + 1)(2\ell + 3)^2(2\ell + 5)} - \frac{2z^6}{(2\ell + 1)(2\ell + 3)^3(2\ell + 5)(2\ell + 7)} - \frac{(10\ell + 27)z^8}{(2\ell + 1)(2\ell + 3)^4(2\ell + 5)^2(2\ell + 7)(2\ell + 9)} - \dots \right]. \tag{33}$$

As is seen from the consideration of series (33), its convergence is better than of series (2). The condition of correct computation of the series is the inequality

$$2\ell > |z|. \tag{34}$$

The difficulty of its use is in the absence of analytical form for the consequent terms. At the same time it is known¹⁰ [and it directly follows from Eq. (10b)] that the backward recurrence for R_ℓ is equivalent to the infinite continued fraction, usually written in the form¹⁵

$$R_\ell(z) = a_0 + \frac{b_1}{a_1 + \frac{b_2}{a_2 + \frac{b_3}{a_3 + \dots}}}, \quad (35)$$

where

$$a_k = \frac{2\ell + 2k + 1}{z}; \quad b_k = -1.$$

The recurrent equations for continued fractions

$$\begin{aligned} P_n &= a_n P_{n-1} + b_n P_{n-2}; \\ Q_n &= a_n Q_{n-1} + b_n Q_{n-2} \end{aligned} \quad (36)$$

with the initial conditions

$$b_0 = 1, \quad P_{-2} = 0, \quad P_{-1} = 1, \quad Q_{-2} = 1, \quad Q_{-1} = 0$$

define the numerator and denominator of the irreducible n th convergent fraction

$$\delta_n = P_n / Q_n \quad (37)$$

which is equivalent to the finite continued fraction free of all terms with $k > n$; the difference of two neighboring convergent fractions is defined by the equation

$$\delta_n - \delta_{n-1} = \frac{(-1)^{n-1} b_1 \dots b_n}{Q_{n-1} Q_n}. \quad (38)$$

One of the criteria for δ_n convergence to a finite limit at $n \rightarrow \infty$ for real b_n and a_n (a_n is positive) after some n_0 is satisfaction of inequalities¹⁵

$$a_n - |b_n| \geq 1, \quad n > n_0. \quad (39)$$

As it follows from Eq. (39), continued fraction (35) converges for real arguments, since $(\ell + k + 1)/x$ always becomes greater than unit with increasing k , i.e., conditions (39) is satisfied. In this case, the question arises about the ratio of which functions Eq. (35) converges to, because Eqs. (35)–(39) formally take place for any Ricatti–Bessel functions. To answer this question, compare the first terms of series (33) for $R_\ell^\psi(z)$ and of the series obtained from division of the multiplier $P_n(z)$ by $Q_n(z)$. To do this, write the expressions for $P_n(z)$ and $Q_n(z)$, obtained from Eqs. (35) and (36):

$$\begin{aligned} P_0 &= \frac{2\ell + 1}{z}, \quad Q_0 = 1; \\ P_1 &= \frac{2\ell + 1}{z} \frac{2\ell + 3}{z} - 1, \quad Q_1 = \frac{2\ell + 3}{z}. \end{aligned} \quad (40)$$

With an increase of the order of convergent fractions, Eqs. (37) and (40) evidently describe more and more terms of series (33). Hence, it may be concluded that infinite fraction (35) converges to $R_\ell^\psi(z)$. To clarify the convergence character, substitute $b_n = -1$ into Eq. (38):

$$R_{\ell,n} - R_{\ell,n-1} = -\frac{1}{Q_{n-1} Q_n}. \quad (41)$$

It is seen from Eq. (36), that at $x \leq 2(\ell + k + 1)$ all $Q_n > 0$, i.e., the difference between two neighboring convergent fractions is negative. This means that the sequence $R_{\ell,n}$ monotonically decreases with increase of n . The difference between R_ℓ and $R_{\ell,n}$ with accounting for Eq. (41) is expressed in the form

$$R - R_{\ell,n} = -\frac{1}{Q_{n+1} Q_n} \left(1 + \frac{Q_n}{Q_{n+2}} + \frac{Q_n Q_{n+1}}{Q_{n+2} Q_{n+3}} + \dots \right). \quad (42)$$

If $n + \ell > z$, the ratio $Q_{n+k}/Q_{n+k+2} \approx 1/4$ and the sum in parenthesis in Eq. (42) approximately equals to $4/3$, according to the expression for the sum of geometric progression. Therefore, the product $Q_n Q_{n+1}$, obtainable from recurrent computation of numerators and denominators of convergent fractions, can serve for formulating the criteria of the recurrent process termination. Hence, in the worked out algorithm for computing R_ℓ^ψ by Eqs. (36) and (37), which is realized for real arguments in the single-precision subroutine RPSIRE (see the Appendix), the following criterion of the recurrent process termination was used:

$$|Q_k Q_{k-1}| \geq C. \quad (43)$$

To assess C , note that R_ℓ^ψ changes from $\ell/x \approx 1$ at $\ell = \ell_1^\psi$ to $(2\ell + 1)/x$ at $\ell \rightarrow \infty$. Hence, to obtain seven true digits, we can choose $C = 10^6$. Numerical study of C by means of comparison of single- and double-precision computations of R_ℓ^ψ for $x \leq 10^5$ and $1 \leq \ell \leq x + 50$ has shown, that this value of C is sufficient, since at its further increase the accuracy of single-precision computations of R_ℓ^ψ does not enhance. It also follows from the study of results, that the number of recurrence rounds for the chosen C is well described by the equation

$$k = 4 + 3.6x^{1/3} \begin{cases} -0.5(\ell - \ell_{\max}^\psi), & \ell \geq \ell_{\max}^\psi, \\ +(\ell_{\max}^\psi - \ell), & \ell < \ell_{\max}^\psi. \end{cases} \quad (44)$$

The above equation answers the question on the choice of initial values n in the Miller algorithm (Ref. 4, p. 270), where $\psi_{\ell+n+1}(z)$ is equal to zero and $\psi_{\ell+n}(z)$ – to unit. As it follows from the comparison of Eqs. (6) and (35), this algorithm is actually equivalent to the direct calculation of the n -convergent continued fraction. Therefore, for 24-bit computers n in the Miller algorithm should be equal to k from Eq. (44). But there is no need in the Miller algorithm

for $\psi_\ell(z)$ due to the new algorithm, suggested in this work. The advantage of the new algorithm is automated determination of k ; the computation of RB3 function is comparable in amount of operations with the computation of the series when normalizing in the Miller algorithm.

In the Lentz algorithm,¹² the procedure of convergent fractions computation includes the recurrent computation of the ratios

$$RP_k = P_k/P_{k-1} \text{ and } RQ_k = Q_k/Q_{k-1},$$

which are easily obtained from Eq. (36) and, therefore, are not given here. The next convergent fraction results from the preceding one:

$$\delta_k = \delta_{k-1} \frac{RP_k}{RQ_k}. \quad (45)$$

In this case, the recurrence termination criterion is the equality of RP_k and RQ_k with the computer accuracy. Note, than one additional operation of multiplication or division takes place at each step of this procedure, which increases the computation time. There is a probability of division by zero in this algorithm, which is excluded in Ref. 12 by a special procedure. To compare the RPSIRE subroutine with the Lentz algorithm, a corresponding program was written without the above procedure for excluding division by zero. It turned out, that the equality of RP_k and RQ_k can not be satisfied when the program¹² running, therefore the equation

$$\frac{|RP_k - RQ_k|}{RQ_k} \leq \varepsilon \quad (46)$$

was used to stop the recurrence process.

A lowest error at single precision was provided by $\varepsilon = 10^{-6}$. In this case, the number of recurrences and computation error virtually equaled to those for RPSIRE at $C = 10^6$, however, the computation time, averaged over the range $x = 10 \div 1000$, was twice as shorter.

Conclusion

The analytical study and numerical results confirm the general stability principle of difference schemes to obtain solutions increasing at their application. According to this principle, absolutely stable for the forward recurrence are the functions $\chi_\ell(x)$ of real and $\eta_\ell(z)$ of complex arguments and the functions $\psi_\ell(x)$ of real argument up to $\ell = \ell_{\max}^{\psi}$, defined by Eq. (16). With further increase of ℓ , the recurrence becomes absolutely unstable and results in generating the sum of $\psi_\ell(x)$ and $\chi_\ell(x)$. The backward recurrence for $\psi_\ell(x)$ is absolutely stable at $\ell > \ell_{\max}^{\psi}$ and relatively stable at $\ell < \ell_{\max}^{\psi}$. In case of complex argument, the backward recurrence stability increases throughout the ℓ range.

When using recurrence procedures in the domains of stability, the basic computation error of functions with decimal arguments occurs due to errors of arguments conversion to the binary system.

To obtain the initial values for the backward recurrence, we suggest to use the ratio $RPSI = \psi_{\ell-1}(z)/\psi_\ell(z)$ and the forward-recurrence computed $\chi_\ell(x)$ or $\eta_\ell(z)$. With the use of Wronskians, this results in Eqs. (20) and (30). To compute RPSI, the continued-fractions procedure is effective, the simplified scheme of which is justified and given in the form of subroutine in this work.

APPENDIX

The subroutine RPSIRE (ratio psi real E) serves for computation the Ricatti–Bessel function of the first kind $RPSI = \psi_{\ell-1}(z)/\psi_\ell(z)$ for real arguments. Change to complex arguments is carried out by simple redescription of variables, at which Eq. (43) remains valid. Input parameters of the subroutine are the order L and the value x , output one is the value of RPSI function.

```

SUBROUTINE RPSIRE(L,X,RPSI)
DX=2./X
W=(L+0.5)*DX
P2=1.
P1=W
Q2=0.
Q1=1.
DO 1 K=2,9999
DX=-DX
W=DX-W
P=W*P1+P2
Q=W*Q1+Q2
IF(ABS(Q*Q1).GE.1.E+6) GO TO 2
P2=P1
Q2=Q1
P1=P
1 Q1=Q
2 RPSI=P/Q
END

```

References

1. H.C. van de Hulst, *Light Scattering by Small Particles* (Wiley, New York, 1957).
2. D. Deirmendjian, *Electromagnetic Waves Scattering on Spherical Polydispersions* (American Elsevier, New York, 1969).
3. C.F. Bohren and D.R. Huffman, *Absorption and Scattering of Light by Small Particles* (Interscience–Wiley, New York, 1986).
4. *Guide in Special Functions*, M. Abramovits and I. Stigan, eds. (Nauka, Moscow, 1979), 832 pp.
5. A.A. Akulinin, *Atmos. Oceanic Opt.* **1**, No. 6, 127–129 (1988).
6. A.A. Akulinin, *Review of some calculation schemes of optical parameters of electromagnetic scattering by a single homogeneous spherical particles*, Dep. VINITI. 16.04.1987, No. 3388–B87.

7. Yu. Luck, *Special Mathematic Functions and their Approximations* (Mir, Moscow, 1980), 608 pp.
8. G.W. Kattawar and G.N. Plass, *J. Opt. Soc. Am.* **6**, No. 8, 1377–1382 (1967).
9. W.J. Wiscombe, *Appl. Opt.* **19**, No. 9, 1505–1509 (1980).
10. I.B. Gavris, *Vestn. BGU, Ser. 1*, No. 3, 8–16 (1974).
11. N.P. Romanov, *Trudy IEM, Is. 45 (135)*, 3–40 (1987).
12. W.J. Lentz, *Appl. Opt.* **15**, No. 3, 668–671 (1976).
13. E.Z. Lubimskii, V.V. Martynuk, and N.P. Trifonov, *Programming* (Fizmatgiz, Moscow, 1980), 608 pp.
14. N.N. Belov, *Atmos. Oceanic Opt.* **5**, No. 2, 107–109 (1992).
15. B.P. Demidovich and I.A. Maron, *Grounds for Computational Mathematics* (Fizmatgiz, Moscow, 1960), 660 pp.