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Coulomb and Bessel Functions of Complex Arguments and Order

I. J. THOMPSON*

Science and Engineering Research Council, Daresbury Laboratory, Daresbury, Warrington WA4 4AD, United Kingdom

AND

A. R. BARNETT

Department of Physics, Schuster Laboratory, University of Manchester, Manchester M13 9PL, United Kingdom

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The coulomb wavefunctions, originally constructed for real $\rho > 0$, real η and integer $\lambda \geqslant 0$, are defined for ρ, η, and λ all complex. We examine the complex continuation of a variety of series and continued-fraction expansions for the Coulomb functions and their logarithmic derivatives, and then see how these expansions may be selectively combined to calculate both the regular and irregular functions and their derivatives. The resulting algorithm [46] is a complex generalisation of Steed's method [6, 7] as it appears in the real procedure COULFG [10]. Complex Whittaker, confluent hypergeometric and Bessel functions can also be calculated. © 1986 Academic Press, Inc.

1. INTRODUCTION

The Coulomb wavefunctions $F_\lambda(\eta, \rho)$ and $G_\lambda(\eta, \rho)$ are the two linearly independent solutions of the differential equation

$$f''(\rho) + (1 - 2\eta/\rho - \lambda(\lambda+1)/\rho^2)\, f(\rho) = 0 \tag{1.1}$$

that are defined by the boundary conditions

$$F_\lambda(\eta, \rho = 0) = 0 \qquad \text{(regular solution)}$$

and

$$F_\lambda(\eta, \rho) \xrightarrow[|\rho| \to +\infty]{} \sin \theta_\lambda,$$

$$G_\lambda(\eta, \rho) \xrightarrow[|\rho| \to +\infty]{} \cos \theta_\lambda,$$

* Present Address: Department of Engineering Mathematics, University of Bristol, Bristol, U.K.

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where $\theta_\lambda = \rho - \eta \ln 2\rho - \lambda\pi/2 + \sigma_\lambda(\eta)$, and *all variables are complex* unless otherwise stated. The quantity σ_λ is the Coulomb phase shift, constructed so that for real $\rho, \eta,$ and λ, the functions F_λ and G_λ are all real; the formula for σ_λ will be given below. The combinations $H_\lambda^\pm = G_\lambda \pm iF_\lambda$ are defined, and become $e^{\pm i\theta_\lambda}$ as $|\rho| \to \infty$ asymptotically.

The real functions F_λ, G_λ, F'_λ, and G'_λ (where the prime indicates $d/d\rho$) have been extensively studied and two main methods of calculation have been developed. The approach exemplified by the reviews of Fröberg [1] and of Hull and Breit [2], and the programs of Bardin *et al.* [3] and of Strecok and Gregory [4], is to divide the ρ, η plane into regions in which suitable transformations of Eq. (1) yield convergent series or integrals. Results for different (integer) λ are obtained by downward (F_λ) and upward (G_λ) recurrence, terminating always at $\lambda = 0$. The approach of Gautschi [5] and of Barnett *et al.* [6–8] makes use of continued fractions and a normalising condition; Gautschi's method yields the regular solution from some λ to $\lambda = 0$ whereas Barnett adopted Steed's more general technique to calculate the regular and irregular functions (with their derivatives) for any specified (real) λ [9] or for a range of integer-spaced λ-values [10]. It is this method which is generalised in the present paper, for it has the remarkable property that no knowledge of the form of the singularity of G_λ at the origin is required.

It is worth emphasising that, due to the normalisations chosen, only Steed's method is suitable for *real* values of λ as opposed to integer values, and indeed for a *single* real value (i.e., obtained without recursion). Such a program is KLEIN [9] which is thus suitable for precise calculations involving the Klein–Gordon equation, the Dirac equation [11, 13] and the Fourier–Bessel equation [13] and many others, e.g., cylindrical and spherical Bessel functions of real order. The present paper is concerned with the extension of not only λ to the complex plane but of the arguments ρ and η as well.

Fröberg's review [1] in 1955 and the monumental survey article by Hull and Breit [2] treat the repulsive potential, real ρ and integer λ values, while that of Curtis [14] in 1964 dealt with the attractive potential, both real and imaginary ρ (positive and negative energies) and gave tables for $\lambda = 0, 1, 2$. Tabular results and a summary of formulae are given by Abramowitz in two articles [17]. A survey paper by Kölbig [15] in 1972 drew attention to the method and program (for repulsive potentials and real ρ) of Gautschi [5] which calculates both F_λ and F'_λ for integer λ, while Fullerton's bibliography [16] of the recent literature appeared in 1980. The most recent review, covering *real* arguments and hence both attractive ($\mathrm{Re}\,\eta < 0$) and repulsive potentials ($\mathrm{Re}\,\eta > 0$), is that of Barnett [8] in 1982; it summarizes and evaluates Steed's continued-fraction method and it provides a detailed comparison between the methods of Gautschi and Steed.

There are relatively few computations and programs available for complex values of the arguments, and these often deal with limited ranges of parameter values. For purely imaginary ρ and η ($= ik$), Whittaker functions were tabulated by Hebbard and Robson [18] for the repulsive potential (when $k < 0$) and by Curtis [14] (when $k > 0$). Two recent programs, designed for electron scattering calculations,

are those of Bell and Scott [19] and of Seaton [20]. Bell and Scott compute Whittaker functions by a combination of an asymptotic expansion and one about the origin; Seaton uses an expansion about the origin and deals with real ρ and with imaginary ρ; and both are limited to relatively few integer λ values ($\lambda < 10$). The recent program of Noble and Thompson [21] extends this λ range and makes use of Padé acceleration methods to improve the convergence of the asymptotic form; both attractive and repulsive fields are solved. Two further programs based on asymptotic expansions for repulsive potentials are those of Tamura and Rybicki [22] for complex ρ (complex energy) and of Takemasa *et al.* [23] for complex λ but real ρ.

Studies in pion scattering and in pionic and kaonic atom energy levels at times require results for complex ρ and complex λ. The papers of Atarashi *et al.* [24], Cooper *et al.* [25], and Rawitsher [26] illustrate different approaches to the question of obtaining sufficient accuracy.

The methods detailed in the present paper will allow the accurate calculations of complex Coulomb functions for every one of the above cases as well as for complex Bessel functions. A detailed survey of comparative calculations is given in a related paper [27] by the authors which serves as a verification of the accuracy claims for the quoted parameter ranges and which demonstrates the comprehensiveness and power of the current approach.

2. Definitions and Analytic Continuation of the Coulomb Functions

Although originally defined for the scattering of charged particles in quantum mechanics, the Coulomb functions F, G, H^+, and H^- can be used to give two linearly independent solutions of *any* second-order differential equation of the form $f'' + g(\rho) \cdot f(\rho) = 0$ where $g(\rho)$ has ρ^{-2}, ρ^{-1}, and ρ^0 terms. If $\eta = 0$, for example, they are simply related to the cylindrical Bessel functions J, Y, $H(1)$, $H(2)$, I, K, and also to the spherical Bessel functions j, y, $h(1)$, and $h(2)$, by

$$J_\nu(\rho) = (2/\pi\rho)^{1/2} F_{\nu-1/2}(0, \rho) \tag{2.1a}$$

$$Y_\nu(\rho) = -(2/\pi\rho)^{1/2} G_{\nu-1/2}(0, \rho) \tag{2.1b}$$

$$j_\nu(\rho) = \rho^{-1} F_\nu(0, \rho) \tag{2.1c}$$

$$y_\nu(\rho) = -\rho^{-1} G_\nu(0, \rho). \tag{2.1d}$$

For integer ν these are standard definitions, given in [17a, Eqs. 14.6.6].

In order to make the analytic continuation of the F and H^ω ($\equiv H^\pm$) Coulomb wavefunctions to each complex plane, with cuts (if present) along the negative real ρ axis, we start [17a, Eqs. 14.1.3 and 14.5.9] with the following hypergeometric series expansions

$$F_\lambda(\eta, \rho) = \rho^{\lambda+1} e^{i\omega\rho} C_\lambda(\eta)\ {}_1F_1(a; b; z) \tag{2.2a}$$

$$H^\omega_\lambda(\eta, \rho) = e^{i\omega\theta_\lambda}\ {}_2F_0(1 + a - b, a;; -1/z) \tag{2.2b}$$

$$= e^{i\omega\theta_\lambda} z^a U(a, b, z) \tag{2.2c}$$

where $a = 1 + \lambda + i\omega\eta$, $b = 2\lambda + 2$, $z = -2i\omega\rho$ and where $\omega = +1$ or -1. ${}_1F_1(a; b; z)$ is alternatively written $M(a, b, z)$. In (2.2a) either $\omega(\pm 1)$ may be chosen (Kummer's transformation) for the best numerical convergence and $C_\lambda(\eta)$ is given by (2.3b). The ${}_2F_0(a, b;; u)$ function has a cut along the real axis from $u = 1$ to $u = \infty$, so (2.2b) can only be used for $-\pi/2 < \omega\arg(\rho) < \pi$.

For η and λ complex in general, the Coulomb functions are related to the Whittaker functions $W_{\chi,\mu}(z)$, which provide another general characterisation [32] of the solutions to (1.1) as $W_{\chi,\mu}(z)$ and $W_{-\chi,\mu}(-z)$. The relation is given through (2.2c) and (13.1.33) of [17a]. Any one of the Coulomb, Whittaker, or hypergeometric pairs of functions could be used as a numerical basis for calculating whichever form may be required. With ω such that $|H^\omega|$ is the smaller of $|H^+|$ and $|H^-|$ we have chosen to use the Coulomb functions F and H^ω as a basis for the following reasons:

1. The Coulomb functions have unit Wronskian $F'H - H'F = 1$, so that F and H will neven both become vanishingly small. This is in contrast to the hypergeometric Wronskian

$$M'U - U'M = -\frac{\Gamma(b)}{\Gamma(a)}\frac{e^z}{z^b}.$$

2. The value of ω is chosen so that the basis pair (F, H^ω) always includes the function in the set $\langle F, G, H^+, \text{and } H^- \rangle$ with the *smallest* modulus (i.e., H^ω when $|\lambda|$ is small and F when $|\lambda|$ is large). This is necessary as that member cannot be accurately calculated by any difference formula. Using Whittaker functions would prevent accurate calculation of F for large $|\lambda|$, since $|F_\lambda|$ becomes small and both the Whittaker functions have large modulus.

3. F and $H^{(\omega)}$ satisfy the same recurrence relations, so that the stability when recurring in a certain direction can be monitored, as any error introduced will behave in proportion to the other solution. This means that recurrence will be stable provided the wanted solution is not decreasing monotonically. This is in contrast to $W_{\chi,\mu}(z)$ and $W_{-\chi,\mu}(-z)$, which satisfy *different* recurrence relations, and for which such a simple guide to stability is not available.

4. It is only a minor disadvantage that the requirement of a unit Wronskian leads to additional square roots in the Coulomb phase shifts and Gamow factors (see below), and that these factors may have poles and zeros for various λ and η combinations (and hence for all ρ for these combinations). The square root ambiguities may be simply resolved by using an analytic log-gamma function with a well-defined cut. It is also easy to return the next-order coefficients of the functions around the poles and zeros to enable, e.g., Whittaker functions to be everywhere reconstructed to full accuracy.

The usual formulae [2] for the Coulomb phase shift $\sigma_\lambda(\eta)$ and Gamow factors $C_\lambda(\eta)$ are given (for integer $\lambda = L$) in [17a, (14.5.6) and (14.1.7), respectively], but

$$\sigma_L = \arg\Gamma(L+1+i\eta) \qquad C_L(\eta) = \frac{2^L e^{-\pi\eta/2}|\Gamma}{\Gamma(2L+2)}$$

these must be analytically continued [28, 29] to the case when λ and η are complex. We use instead

$$\sigma_\lambda(\eta) = [\ln \Gamma(1+\lambda+i\eta) - \ln \Gamma(1+\lambda-i\eta)]/(2i) \tag{2.3a}$$

and

$$C_\lambda(\eta) = 2^\lambda \exp\{-\pi\eta/2 + [\ln \Gamma(1+\lambda+i\eta) + \ln \Gamma(1+\lambda-i\eta)]/2 - \ln \Gamma(2\lambda+2)\} \tag{2.3b}$$

Consistent procedures must be given to determine the multiple of $2\pi i$ in the complex logarithms. Following Kölbig [15, 30], we define an analytic log-gamma procedure $\ln \Gamma(w)$ with its cut along the negative real w-axis. This function is therefore single-valued for all w not on the cut (where it changes discontinuously by a multiple of $2\pi i$). The above $\sigma_\lambda(\eta)$ and $C_\lambda(\eta)$ are thus well defined everywhere except on the cut, and are mutually consistent according to

$$C_\lambda(\eta) = 2^\lambda \exp(-\pi\eta/2 - i\omega\sigma_\lambda)\, \Gamma(a)/\Gamma(b). \tag{2.4}$$

This consistency procedure means that even if a ($=1+\lambda+\omega i\eta$) *is* on its cut (i.e., is non-positive real), the uncertainty of $2\pi i$ in the $\ln \Gamma$ function only changes the *sign* of all the C_λ, $e^{i\sigma}\lambda$, F, and H^ω *simultaneously*, so that formulae (2.2) for the hypergeometric and Whittaker functions still hold. The M, U, and W functions are all continuous in the neighbourhood of the cuts.

3. Expansions Suitable for Numerical Calculation

The F and H^ω basis functions are defined, (2.2), through the hypergeometric series expansions

$${}_1F_1(a;b;z) = 1 + \frac{a}{b}\frac{z}{1!} + \frac{a(a+1)}{b(b+1)}\frac{z^2}{2!} + \cdots \qquad \text{with} \quad z = -2i\omega\rho \tag{3.1}$$

and

$${}_2F_0(a;b;;u) = 1 + \frac{abu}{1!} + \frac{a(a+1)\,b(b+1)\,u^2}{2!} + \cdots \qquad \text{with} \quad u = \omega/(2i\rho) = -1/z \tag{3.2}$$

which can be used directly only for small $|\rho|$ and large $|\rho|$, respectively, so there is an intermediate range where neither is adequate on its own. In this middle region round-off errors in the partial sums of the ${}_1F_1$ series are large fractions of the final value, and with the ${}_2F_0$ asymptotic expansion the terms start increasing again before sufficient accuracy has been obtained. As it is absolutely convergent, the

accuracy of the ${}_1F_1$ series can be improved by selective extended-precision arithmetic, but there are still intermediate regions requiring different treatments.

These are problems which faced the authors of programs exploiting these formulae; for example, Towner and Hardy [12] in an unpublished program to evaluate U and M and hence β-decay integrals in nuclear physics and Moon [31] in a program to calculate Airy functions [$\lambda = -1/6$, $\eta = 0$, complex ρ].

There are three principal means of improving the range of allowable arguments:

(1) using recurrence relations,

(2) calculating logarithmic derivatives F'/F and $H^{\omega\prime}/H^{\omega}$,

(3) using Padé acceleration via continued fractions.

These extensions may be verified either by (3.1), (3.2), or by comparison with the integral representations (14.3.1) and (14.3.3) for the irregular solution of [17a]. We used the adaptive integrator D01AKF from the NAG library, choosing that integral which was calculated most accurately. Such verifications were necessary because no previously published procedure finds the Coulomb functions when ρ, η, and λ are all complex.

3.1. *Recurrence Relations*

The F, G, and H^{ω} functions all satisfy the same three-term relation

$$R_\lambda U_{\lambda-1} = T_\lambda U_\lambda - R_{\lambda+1} U_{\lambda+1} \tag{3.3}$$

alternative forms of which are

$$R_\lambda U_{\lambda-1} = U'_\lambda + S_\lambda U_\lambda$$

and

$$U'_{\lambda-1} = S_\lambda U_{\lambda-1} - R_\lambda U_\lambda,$$

where

$$S_\lambda = \lambda/\rho + \eta/\lambda, \qquad T_\lambda = S_\lambda + S_{\lambda+1},$$

and

$$R_\lambda = (2\lambda+1)\, C_\lambda(\eta)/C_{\lambda-1}(\eta) \qquad (\text{so } R_\lambda^2 = 1 + \eta^2/\lambda^2) \tag{3.4}$$

for $U_\lambda = F_\lambda$, G_λ, H_λ^+, or H_λ^-. These can be rearranged for upward recurrences, i.e., increasing $\Lambda \equiv \mathrm{Re}(\lambda)$.

Calculation by recurrence is numerically stable provided the desired function is not monotonically decreasing. This simple criterion for determining the stable direction relies on the wanted and unwanted solutions having a Wronskian independent

of λ. This is not the case for direct recursion of the Whittaker functions, for although $W_{\chi,\mu}(z)$ and $W_{-\chi,\mu}(-z)$ have λ-independent Wronskians, they *recur using different relations*. Thus the unwanted solution in the recursion of, say, W^+, is not W^- but some other function whose Wronskian with W^+ *does* depend on λ, and examples exist of W^+ recurrences being unstable even though it monotonically increases. Consider the behaviour for the case $\rho = 37.5i$, $\eta = 6.67i$ for λ increasing from 0–15 as is given in Bell and Scott [19]. The errors here grow by 10 orders of magnitude as [27] demonstrates.

In order to determine the directions of stable recurrence of a particular Coulomb function, we need only see where the modulus of that function either oscillates or increases monotonically. We retain the nomenclature used when λ is real, i.e., upward recurrence implies Λ increases in integer steps and downward recurrences implies Λ decreases in integer steps.

For large Λ the regular solution F_λ is the only minimal function [5]

$$(\lim_{\Lambda \to \infty} F_\lambda / H_\lambda = 0 \text{ for any } H_\lambda \text{ not linearly dependent on } F_\lambda)$$

so downward recurrence of F_λ from large Λ is stable down to some turnover point after which $|F_\lambda|$ may decrease. Indeed for F_λ the stronger condition

$$\lim_{\Lambda \to \infty} F_\lambda = 0$$

holds. Conversely, the H^ω and G all have mixtures of the irregular solution, so their upward recurrence is stable for Λ above the same turnover point.

For λ near zero, the H^ω solutions behave as $e^{i\omega\theta_\lambda}$, so when θ_λ has a significant imaginary component, one of the $|H^\omega|$ will be small and $H^{-\omega}$, F and G will all have large modulus. As H^ω is small for small Λ, and (from the above) large as $\Lambda \to \infty$, upward recurrence of H^ω will be stable—provided we check that it does not decrease for a while before increasing asymptotically.

The adopted procedure is therefore to recur F_λ downward and H^ω_λ upward, calculating $H^{-\omega}_\lambda$ and G_λ from them at each λ, but reversing both these directions if, for a range at low $|\lambda|$-values, $|F_\lambda|$ increases and $|H^\omega_\lambda|$ decreases with increasing $|\lambda|$. This reversal occurs, for example, for bound states in attractive Coulomb potentials for λ from 0 up to $\sqrt{-\eta\rho}$.

Note that when recurring in the region $\Lambda \leqslant -1$ the regular and irregular solutions are remixed, and the increasing and decreasing behaviour of the moduli can become quite complicated. A much more reliable way of finding the functions for Λ negative is to express them in terms of the functions for $\lambda' = -\lambda - 1$. This is because for λ and λ' the values of $\lambda(\lambda+1)$ are equal, and the functions satisfy the same differential equation and differ only in their boundary conditions. The Coulomb phase shifts σ_λ and σ'_λ are known by (2.3a), so

$$H^\omega_\lambda = H^\omega_{\lambda'} \exp(i\omega\chi) \tag{3.5a}$$

where

$$\chi = \sigma_\lambda - \sigma_{\lambda'} - (\lambda + \tfrac{1}{2})\,\pi. \tag{3.5b}$$

3.2. *Logarithmic Derivatives*

In principle it should be easier to calculate the ratios F'/F and $H^{\omega\prime}/H^{\omega}$ than the functions F and H^{ω} themselves because divergences in the function evaluations only affect the ratios in second order. The most important advantages however, are that for these ratios there exist continued-fraction expansions with coefficients given by simple algebraic expressions, and that there exist several methods (see Appendix) for the progressive evaluation of the continued fractions to the required accuracies.

3.2.1. *Continued Fraction CF1 for the Regular Solution*

The first continued fraction, CF1, calculates the logarithmic derivative at the regular solution $F_\lambda(\eta, \rho)$ as

$$\mathrm{CF1} \equiv \frac{F'_\lambda}{F_\lambda} = S_{\lambda+1} - \frac{R^2_{\lambda+1}}{T_{\lambda+1} -} \frac{R^2_{\lambda+2}}{T_{\lambda+2} -} \frac{R^2_{\lambda+3}}{T_{\lambda+3} - \cdots} \tag{3.6}$$

and is essentially [8] the recursive evaluation of (3.3) in the form

$$F_{\lambda+1}/F_\lambda = R_{\lambda+1}/[T_{\lambda+1} - R_{\lambda+2}F_{\lambda+2}/F_{\lambda+1}]$$

up to a large $\Lambda = M$, say.

CF1 is therefore accurate to the required tolerance ε if and only if Miller's downward recurrence from F_m is sufficiently stable ($m = M + i\,\mathrm{Im}\,\lambda$), and by Section 3.1 this depends on $|F_\lambda|$ not decreasing monotonically in any significant region from $\Lambda = M$ towards to the desired λ. This is not always true, as sometimes $|F_\lambda|$ increases with increasing Λ before decreasing asymptoticaly as $\Lambda \to \infty$, so CF1 will not always be accurate. This is the same anomalous case that was noted in Section 3.1. Indeed, if $|F_\lambda|$ increases by more than $\varepsilon^{-1/2}$ then CF1 will pick up the decreasing H^{ω} solution, and may give the wrong sign for the logarithmic derivative. CF1 is also unstable for λ near to a negative integer, but the reflection rules could well be used in these cases.

3.2.2. *Continued Fractions CF2(ω) for the Irregular Solutions*

The second continued fraction calculates the logarithmic derivative of H^+_λ or H^-_λ as,

$$\mathrm{CF2}(\omega) \equiv \frac{H^{\omega\prime}_\lambda}{H^{\omega}_\lambda} = i\omega(1 - \eta/\rho) + \frac{i\omega}{\rho} \cdot \frac{ac}{2(\rho - \eta + i\omega) +} \frac{(a+1)(c+1)}{2(\rho - \eta + 2i\omega) + \cdots}$$

where $a = 1 + \lambda + i\omega\eta$ and $c = -\lambda + i\omega\eta = 1 + a - b$, and is based [6, 8] on the recursive evaluation of the inverse of the ratio

$$\frac{{}_2F_0(a; c;; u)}{{}_2F_0(a+1, c+1;; u)} = 1 - (a+c+1)\,u - u^2(a+1)(c+1)\frac{{}_2F_0(a+2, c+2;; u)}{{}_2F_0(a+1, c+1;; u)}$$

(it is equivalently the odd contraction of Gauss' continued fraction for ${}_2F_0$ [33, 34]). Although the ${}_2F_0$ series is only asymptotically convergent, this ratio has a very strong convergence property, and the continued fraction is convergent throughout the complex u-plane exterior to the ${}_2F_0$ cut along the real axis from $u = 1$ to $u = \infty$. The CF2(ω) is therefore convergent except when ρ approaches the line joining the origin to $u = -i\omega/2$, where it changes discontinuously, and thus is convergent everywhere on the side of real ρ axis, where H^ω tends to be exponentially decreasing. In contrast to the evaluation of CF1, no instabilities have been detected, and for $|\rho| > 10^{-3}$ the CF2 is found to be numerically accurate to within several digits of machine accuracy even though the number of terms required for convergence rises approximately as $|\rho|^{-0.75}$ as $|\rho| \to 0$. For $|\rho| \ll 1$, the methods of Section 3.2.5 are more efficient.

On the side of the real axis opposite to the cut, i.e., for $\mathrm{Im}(\rho) < 0$ for CF2$^+$ as shown in Fig. 1, the CF2 only gives $H^{\omega\prime}/H^\omega$ correctly for $\mathrm{Re}(\rho) > 0$. This is because H^ω changes discontinuously on its cut placed on the negative ρ axis by definition, but CF2 does not suddenly change there. Therefore, even though the CF2(ω) are convergent in all quadrants, they can only be used for $-\pi/2 < \omega \arg(\rho) < \pi$, and in the remaining quadrant different methods must be used.

3.2.3. *Asymptotic Expansions for the Regular Function*

An asymptotic expression exists for the logarithmic derivative F'_λ/F_λ, which we call CF1A as it is based on the asymptotic expansions for H^+ and H^-:

$$\mathrm{CF1A} \equiv (H^{+\prime} - H^{-\prime})/(H^+ - H^-) = \lim_{N \to \infty} h_N \tag{3.8}$$

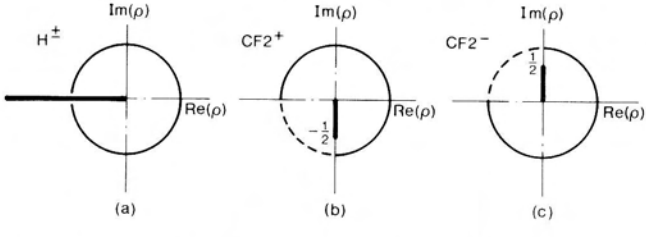

FIG. 1. Analytic ranges and cut positions of the logarithmic derivatives of $H^\pm$ and the continued fractions CF2$^+$ and CF2$^-$. In the dashed quadrants, CF2$^\pm$ do not equal the logarithmic derivatives of $H^\pm$.

where

$$h_N = \sum_{k=1}^{N} (g_k^* \cos\theta_\lambda + f_k^* \sin\theta_\lambda) \Big/ \sum_{k=1}^{N} (g_k \cos\theta_\lambda + f_k \sin\theta_\lambda).$$

The coefficients g_k^*, f_k^*, g_k, and f_k obey the recurrence relations given in [17a (14.5.8)].

The numerators and denominators are themselves asymptotic expansions for F'_λ and F_λ given by Fröberg [1] and in [17, Eq. 14.5]. They both converge most quickly for large $|\rho|$, but their ratio converges more quickly than the separate expansions.

To use CF1A for still smaller values of $|\rho|$, we must calculate the coefficients of the corresponding continued fraction, and evaluate that continued fraction. This is equivalent to Padé acceleration of the sequence h_N, and is discussed further in Section 3.3.

The validity of CF1A in the complex ρ-plane depends on the ${}_2F_0$ asymptotic expansions for H^+ and H^- *both* being accurate. The expansions for H^ω are valid just where CF2$^\omega$ are valid, and their regions of validity overlap only for $\mathrm{Re}(\rho) \geqslant 0$ except where $\mathrm{Re}(\rho) = 0$ and $|\mathrm{Im}(\rho)| \leqslant \frac{1}{2}$. To extend to the negative $\mathrm{Re}(\rho)$ half-plane, the reflection formula

$$f_\lambda(\eta, \rho) = -f_\lambda(-\eta, -\rho) \tag{3.9}$$

where $f_\lambda \equiv F'_\lambda / F_\lambda$, can be used since the logarithmic derivative of just the regular solution is being calculated.

3.2.4. *Continued Fraction CF1′ for the Regular Solution*

Two more expressions for F'/F exist in continued-fraction form, called CF1′(ω) for $\omega = \pm 1$ as they are similar to CF1, but derived more directly from the defining equation (2.2a) for F_λ. Using one of the continued fractions (66) in the useful catalogues of Wynn [34], i.e.,

$$\frac{{}_1F_1(a+1; b+1; z)}{{}_1F_1(a; b; z)} = \frac{b}{b-z+} \frac{(a+1)z}{b-z+1+} \frac{(a+2)z}{b-z+2\cdots}$$

it follows that

$$\mathrm{CF1}'(\omega) = \frac{\lambda+1}{\rho} - i\omega + \frac{2i\omega a}{b-z+} \frac{2i\omega\rho(a+1)}{b-z+1+} \frac{2i\omega\rho(a+2)}{b-z+2+\cdots} \tag{3.10}$$

with a, b, z as in (2.2).

For small values of $|\rho|$ compared with $|\eta|^2 + |\lambda|$, CF1′(ω) both converge rapidly to the correct result. For larger values of Re ρ, however, CF1′(ω) both suffer from "false convergence" as first pointed out by Gautschi [35]. That is, the differences between successive convergents of CF1′ become small, seeming to indicate con-

vergence, but then increase again by many orders of magnitude before finally converging. This is exactly analogous behaviour to the CF1 instabilities discussed in Section 3.2.1, but now occurs for ρ, η, and λ all real. This in itself is not a serious defect for CF1′—the problem is to determine when it occurs, and to decide which choice of ω value (if either) gives a correct result. The CF1 behaviour is understood as it depends on the recurrence behaviour of $F_\lambda(\eta, \rho)$ values for integer-spaced λ values with η and ρ constant. The CF1′(ω) behaviour, by contrast, depends on the stability of recurring $F_{\lambda+k}(\eta + i\omega k, \rho)$ values downward from a large k to $k=0$ in steps of $\frac{1}{2}$, and as $F_\lambda(\eta, \rho)$ values for differing η parameters are not usually compared, the general behaviour of CF1′ is an open question.

3.2.5. *Expansions of the Irregular Solution about the Origin* $\rho = 0$

The simplest expansion of $G_\lambda(\eta, \rho)$ as an expansion about $\rho = 0$ uses (3.5) to give

$$G_\lambda(\eta, \rho) = [F_\lambda(\eta, \rho)\cos\chi - F_{\lambda'}(\eta, \rho)]/\sin\chi \tag{3.11}$$

where $\lambda' = -\lambda - 1$, and F_λ and $F_{\lambda'}$ are given by the usual ${}_1F_1$ series (2.2a). This is analogous to (13.1.3) of [17a] and is suitable for non-integral λ.

For $\chi = 0$ (i.e., integer λ) (3.11) becomes indeterminate, but its limiting value as $\chi = 0$ may be determined by L'Hôpital's rule. In these cases the irregular solution has a logarithmic singularity at the origin, as shown in (13.1.6) of [17a].

These two expansions of the irregular solution in terms of the regular solutions of positive and negative orders (or the limit of this is 2λ is integral), are often used to define formally the whole irregular solution. These have been suggested as a numerical method [48, 49], especially after expanding the F_λ in terms of $F_{\lambda+k}$ for $k \geqslant 0$, but they are only practical for $|\rho| < 1$. For larger $|\rho|$ there are prohibitive cancellation errors [50]. For $|\rho| < \frac{1}{2}$, however, they usefully supplement CF2, and have the advantage that their cuts can be set correctly on the negative real ρ axis.

3.3. *Padé Acceleration via Continued Fractions*

When a power series in z for a function $f(z)$ diverges because singularities for small z define a small radius of convergence, it would be reasonable to expect rational approximations to the function to be useful for analytic continuation to larger $|z|$ values. Padé methods (see, e.g., [33, 36, 37, 38] can be used to construct these rational approximations. The best-converged members of the Padé table $P_{N,M}$ are usually the diagonal ($N = M$) and near-diagonal ones, and these members are precisely [33, p. 380] the values of successive convergents of the continued fraction constructed to "correspond" to the original power series, by requiring their coefficients to agree up to a certain power z^{N+M} but not above.

For practical calculations there is therefore a wide variety of equivalent methods. The coefficients of the numerator and denominator polynomials may be found explicitly by solving a set of linear equations [37, p. 9] or by the more compact algorithm DFRACT of [39, 55], or their numerical ratios $P_{N,M}$ in the Padé table

may be sequentially evaluated using Wynn's NEWS algorithm, or his ε-algorithm [40, 41]. Alternatively, the diagonal Padé members may be evaluated by means of the corresponding continued fraction, whose coefficients may be found by the QD-algorithm [42], the PD-algorithm [43], or the P-algorithm [44, 45]. These methods all require working arrays of (in total) $4N$ numbers to calculate a fraction of N terms, and take a time rising as N^2.

We find [21] that the Padé acceleration of the asymptotic expansion (3.2) extends the convergence to larger $z = 1/(2i\rho)$, subject only to exponent overflow and to N being sufficiently large. This improvement is more marked than with the power series (3.1), for which Padé acceleration reduces [55] the cancellation errors in the partial sums, but does not significantly extend the radius of convergence.

Because in a practical computation, e.g. [46], the working arrays have a predefined size (in FORTRAN), and because failure to converge in this space consumes considerable effort, it is important to estimate as accurately as possible beforehand whether or not to attempt Padé acceleration of a given series. If the continued fraction CF2(ω) for the logarithmic derivative $H^{\omega\prime}/H^{\omega}$ has already been evaluated, then we can use the emperical relation observed in Fig. 2, which plots the correlations between the number of iterations "NPQ" required for CF2(ω) and

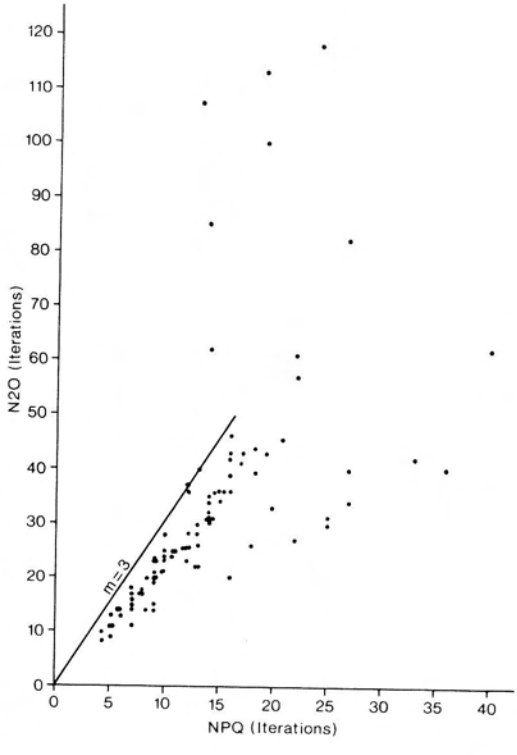

FIG. 2. Correlation of the number of iterations required for CF2 and H^{ω}.

the number "N20" of iterations for a continued-fraction acceleration of the ${}_2F_0$ series for H^{ω} itself. We observe that at least for NPQ < 15, the N20 values are bounded by approximately 3.0 × NPQ. See Case 4, Section 4.2.

3.4. *Temme's Algorithm for the Irregular Solution*

Temme's algorithm [51] yields the absolute normalisation of the irregular solution by means of a sum rule for a sequence of function values evaluated for $i\eta$ differing by unity, all with the same λ value. Recurrence relations connect members of this sequence just as they connect sequences of the same η and differing λ. The sequence for the Temme algorithm can be given as $H_{\lambda}^{\omega}(\eta - ik\omega, \rho)$ for k integral, or equivalently (by 2.2b) as $\Phi_k = {}_2F_0(a+k, c+k;; u)$. The Φ_k satisfy the recurrence relation

$$\Phi_{k-1} = \Phi_k B_k/(2\rho) + \Phi_{k+1} A_{k+1}/(4\rho^2) \tag{3.12}$$

where $A_{k+1} = (a+k)(c+k)$ and $B_k = 2(\rho - \eta + i\omega k)$.

From (3.12) one has the continued fraction

$$\Phi_1/\Phi_0 = \frac{2\rho}{B_1 +} \frac{A_2}{B_2 + \cdots}$$

from which CF2 (3.7) can be immediately derived. Temme shows furthermore than the Φ_k are normalised by

$$\sum_{k=0}^{\infty} C_k \Phi_k = 1 \tag{3.13}$$

where $C_0 = 1$ and $C_k = i\omega C_{k-1} A_k/(2\rho k)$. This sum, and the continued fraction, are both convergent because (as proved in [51]) Φ_k is the minimal solution as $k \to \infty$. This means that Miller's backward-recurrence method [56] can be used to construct the Φ_k (and hence the ratio Φ_1/Φ_0) to any required accuracy provided the downward recurrence is started at a sufficiently large k value.

Campell [52, 53] and Amos [54] use this algorithm for Bessel functions ($\eta = 0$) and use precalculated approximations for the necessary starting orders for Miller's method to reach sufficient accuracy. For a given accuracy approximately 3.5 times as many terms are needed for the sum (3.13) compared with those sufficient for just the (continued fraction) ratio Φ_1/Φ_0. Methods are available, see Appendix, to evaluate the continued fraction forward to any required accuracy, and can be modified [47] to also calculate the sum (3.13) (relative to Φ_0), so avoiding precalculated limitations on accuracy.

Temme's algorithm is formally correct for each of the (ρ, η, λ) complex planes (with the cuts as for CF2; see Fig. 1), but for general η, λ there are often severe cancellations in the sum (3.13). It is only sufficiently accurate however, if [51] b is

restricted to be real and in [0, 1], and a to positive real values. In practice, we find it only useful for $|\lambda + \frac{1}{2}|$ and $|\mathrm{Re}(\eta)|$ both less than unity.

Temme's algorithm appears most suited for purely imaginary η values and for Bessel functions ($\eta = 0$) of real order λ and complex ρ (as in [53, 54, and 47]). For real orders, upward recurrence is always possible from λ_0 satisfying $|\lambda_0 + \frac{1}{2}| \leqslant \frac{1}{2}$ to any required λ. In these restricted regions, Temme's algorithm would be a fast and simple replacement for Padé acceleration of the ${}_2F_0$ series. For complex Coulomb functions, however, the Padé method gives nearly full machine accuracy in those cases where Temme's approach suffers from cancellation errors.

4. Combinations of Methods According to the (ρ, η, λ) Region

We now outline suitable choices of the algorithms of Section 3 in order to calculate the complex Coulomb functions for given ρ, η, λ values and which are embodied in the FORTRAN progam COULCC [46]. In general, accuracies within a few decimals of machine accuracy are possible.

To calculate the basis functions F_λ and H_λ^ω it is sufficient to have their logarithmic derivatives together with some means of absolute normalisation. Recurrence relations can also be used to link λ values with real parts Λ which differ by integers; therefore in the range from $\lambda_{\min}$ to $\lambda_{\max} = \lambda_{\min} + k$, for integral $k \geqslant 0$, the imaginary part of λ remains constant and the case of a single complex λ value ($k = 0$) is included. If such a range of λ-values is required the numerical stability of the recurrence relations demands that the logarithmic derivative of each function should be evaluated at that end of the λ range from which the function does *not* then monotonically decrease in modulus. The regular (minimal) solution is therefore usually recurred with Λ decreasing and the irregular solution with Λ increasing. For a given range of stable recurrences (λ_m, λ_l) the structure of algorithm COULCC is shown in Fig. 3 and is similar to that of the algorithms for real arguments [7, 10].

We now describe how to make the choices

(1) between CF1A and CF1 to compute the logarithmic derivative of the regular solution at λ_l; and,

(2) between the Cases 1–6 of methods for finding the absolute normalisations (using appropriate versions of the Wronskian).

4.1. *Choice of Continued Fraction to Compute F'/F*

Usually the asymptotic form CF1A is simply a quicker method of calculating F'_λ/F_λ for large $|\rho| \gg |\eta|^2 + |\lambda|$, as CF1 takes at least $|\rho|$ iterations for convergence. Procedure COULCC chooses CF1A if $|\rho| > \mathrm{ASYM} \cdot C_{\eta\lambda}$ where $C_{\eta\lambda}$ is a number describing the difficulty for CF1A:

$$C_{\eta\lambda} = (|\mathrm{Re}(A)| + \mathrm{Im}(A)^2 + |\mathrm{Re}(B)| + \mathrm{Im}(B)^2)/2 \tag{4.1}$$

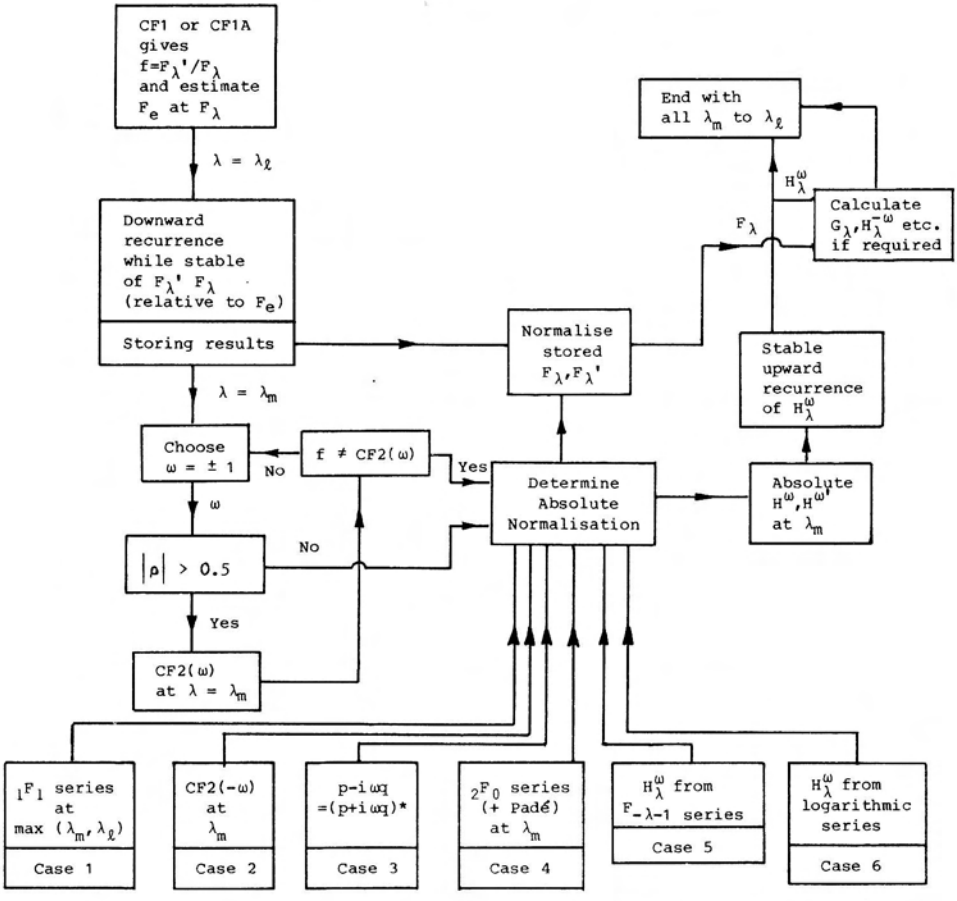

FIG. 3. Flow diagram for the evaluation of the complex Coulomb functions for the λ range λ_m to λ_l.

with $A = 1 + \lambda + i\eta$ and $B = 1 + \lambda - i\eta$ and the parameter ASYM = 3.0. Sometimes however, when CF1 is unstable or λ is near a negative integer then CF1A *must* be used even if it does not fully converge.

4.2. *Cases of Absolute Normalisation*

For all ρ, η, and λ, the regular logarithmic derivative F'/F is available (from above), and also for $|\rho| > 0.5$ the irregular $H^{\omega\prime}/H^{\omega}$ derivative from CF2(ω). The "ω" value has been chosen to minimise the cancellation on the left-hand side of the Wronskian

$$F'/F - H^{\omega\prime}/H^{\omega} = 1/(F \cdot H^{\omega})$$

so the product $F \cdot H^{\omega}$ can be found close to machine accuracy. To find all of F', F, $H^{\omega\prime}$, and H^{ω}, however, a *fourth* input is required: either the CF2$(-\omega)$ derivative, an explicit F or H^{ω} evaluation, or, when ρ, η, and λ are on their real axes, the method of [8, 10] which is Case 3, below. This latter (using the notation $f = F'/F$ and $p + i\omega q = H^{\omega\prime}/H^{\omega}$) gives

$$F = \pm [q/\{(p-f)^2 + q^2\}]^{1/2} \tag{4.2}$$

and

$$H^{\omega} = F[(f-p)/q + i\omega]. \tag{4.3}$$

The six cases in the code COULCC [46] cover the six different possibilities:

Case 1. F from ${}_1F_1$ series (3.1).

Case 2. $p - i\omega q = H^{-\omega\prime}/H^{-\omega}$ from CF2 $(-\omega)$.

Case 3. $p - i\omega q$ from $(p + i\omega q)^*$ (when p and q real).

Case 4. H^{ω} from ${}_2F_0$ expansion (3.2).

Case 5. H^{ω} from F_{λ} and $F_{-\lambda-1}$ (3.11), with F from ${}_1F_1$ series, and not CF2(ω).

Case 6. H^{ω} from logarithmic expression (see Sect. 3.2.5) with F from ${}_1F_1$ series, and not CF2(ω).

To decide which case to employ, we use the following considerations:

Case 1. A direct series evaluation which is used as a last resort.

Cases 2 *and* 3. If $p - i\omega q$ is to be useful, then f, $p + i\omega q$ and $p - i\omega q$ must all be different, so the Wronskians $W(F, H^{\omega})$, $W(F, H^{-\omega})$, and $W(H^{\omega}, H^{-\omega})$ may all be used without significant cancellation errors. This occurs for ρ, η, and λ near their real axes, with $\mathrm{Re}(\rho) > |\rho_{\lambda}|$ (ρ_{λ} is the "turning point" $\eta + \sqrt{(\eta^2 + \lambda(\lambda+1))}$), as then F, H^{ω}, and $H^{-\omega}$ are all oscillatory with moduli around unity. If ρ, η, and λ are *on* their real axes, p and q are real, and Case 3 is most efficient, using (4.2), (4.3) (the method of [10]).

Case 4. The ${}_2F_0$ expansion, with Padé acceleration, is only useful if it converges in the working space available. We use the empirical criterion described in Section 3.3, which is generally satisfied for $|\rho| \gg |\eta|^2 + |\lambda|$.

Cases 5 *and* 6. If $|\rho| < 0.5$, then CF2(ω) converges too slowly, so the four inputs are F'/F, F from the ${}_1F_1$ series, the Wronskian $W(F, H^{\omega})$, and H^{ω} from Section 3.2.5.

Case 1 is important for moderate $|\rho|$ "inside" the turning point $|\rho_{\lambda}|$, and for λ with a large imaginary part. The ${}_1F_1$ series is now evaluated in extended precision to improve the handling of these difficult cases (see Sect. 5).

5. Remaining Regions of Difficulty

For large η or for large $\mathrm{Im}(\lambda)$, there remain problems as the ${}_1F_1$ series may have large rounding errors even in extended precision and the ${}_2F_0$ expansion may not converge even when Padé accelerated. In these cases it is usually difficult to establish the overall normalisation of all the Coulomb functions calculated, but sometimes the problem is more severe because of greater recurrence instabilities for large η. For $\rho = 200i$ and $\eta = 75i$, for example, F_λ increases by 24 orders of magnitude from $\lambda = 0$ to $\lambda = 90$, and so CF1 evaluated at $\lambda < 60$ will give the logarithmic derivative of H not F. The difficulty is that downward recurrence starting from this (wrong) logarithmic derivative will be stable, so the COULCC procedure will not even detect the fact that the near-minimal solution it is calculating is *not* the regular solution. The CF1A expansion should be used therefore if instabilities are even suspected, but if η and λ are too large compared with ρ, then the CF1A will not converge to any useful accuracy, and COULCC must fail. If calculations in such regions are desired, therefore, additional large-η expansions must be employed. Complex generalisations of the Bessel function or Airy-function expansions of [17a], Eqs. 14.4.1–14.4.10 may be useful, along the lines suggested in [29]. These however are most efficient in the $|\eta| \gg |\rho|$ limit, but the above problems occur for $|\eta| \approx |\rho|$. They are also less efficient in general, as the calculation of the Bessel or Airy basis functions requires the calculation of special cases of the Coulomb functions themselves such as by [47, 52, or 54] and the full Coulomb functions might have been calculated without much more effort.

6. Conclusions

The considerations described in Section 4 have been used to construct a FORTRAN routine COULCC, and this program is being published concurrently [46]. It is designed to use the most accurate of Cases 1 to 6 to calculate the regular solution $F_\lambda(\eta, \rho)$, one of the irregular solutions G, H^+, or H^-, and their derivatives for a range of complex orders λ with integer-spaced real parts, Λ. Except for the limitations described in Section 5, the results are accurate to within 2 or 3 decimals of machine accuracy. This performance has been verified for Bessel functions by comparisons [47] with other Bessel codes [53, 54]. Only a few other codes [10, 19, 21] attain similar accuracy for Coulomb functions, while those in [3, 5, 20, 22, or 23] have noticeable accuracy limitations. An error estimate is produced within COULCC by examining cancellations at selected stages of the calculation; the accuracy of this estimate has been also tested (cf. [57]) by the comparison with an extended-precision version of itself.

These routines can optionally produce the Bessel functions J, Y, H, I, or K as they can set $\eta = 0$ and rescale the solutions by (2.1). A simplified Bessel version BESSCC [27] is also being constructed, specialised to real orders $\lambda > -\frac{1}{2}$, to avoid not only the square roots in (3.4) but also the recurrence instabilities of Section 5.

Both COULCC and BESSCC avoid precalculated starting orders for Miller's algorithm [5, 53, 54, 56] by the use of the modified Lentz's method (Appendix III) for the forward evaluation of continued fractions to near machine accuracy. This feature improves the portability of the new codes.

APPENDIX: The Forward Evaluation of Continued Fractions

The problem is to evaluate the convergents

$$h_n = b_0 + \frac{a_1}{b_1+}\frac{a_2}{b_2+}\cdots\frac{a_{n-1}}{b_{n-1}+}\frac{a_n}{b_n}$$

for $n = 1, 2,...$ successively.

(I) The simplest method evaluates $h_n = A_n/B_n$, where A_n and B_n are found from the recurrence relations

$$A_n = A_{n-1}b_n + A_{n-2}a_n$$
$$B_n = B_{n-1}b_n + B_{n-2}a_n$$

starting with the initial conditions $A_{-1} = 1$, $A_0 = b_0$, $B_{-1} = 0$, $B_0 = 1$. However, the A_n and B_n tend to grow exponentially with n, and usually need to be tested for overflow and renormalised when necessary.

(II) Steed's method [6] does not use A_n and B_n explicitly but only the ratio $D_n = B_{n-1}/B_n$. It calculates D_n and $\Delta h_n = h_n - h_{n-1}$ recursively using $D_n = 1/(D_{n-1}a_n + b_n)$ and $\Delta h_n = (b_n D_n - 1)\,\Delta h_{n-1}$. However, it can occasionally happen that $D_{n-1}a_n + b_n \approx 0$, so that D_n and Δh_n will be very large. The next Δh_{n+1} will typically cancel this large change, but only with some loss of accuracy in the numerical running sum $h_{n+1} = \sum \Delta h_m$. This failure occurs, for example, when calculating CF1 for $\lambda = \eta = 0$ and $\rho = \sqrt{15}$.

(III) Lentz's method [58] uses both the ratios $D_n = B_{n-1}/B_n$ and $C_n = A_n/A_{n-1}$, and it calculates the *ratio* $\Delta_n = h_n/h_{n-1}$ of successive convergents. This allows h_n to be large in the above cases, but enables $h_{n+1} = \Delta_{n+1}h_n$ to be calculated without further loss of accuracy. It is now only necessary to avoid divisors being exactly zero (i.e., less than machine precision), by shifting them to, e.g., 10^{-50} if necessary. We therefore recommend Lentz's method (modified to include these zero shifts) as both avoiding exponent overflows and yielding results of uniform accuracy. In full, the method for the evaluation of $h = \lim_{n\to\infty} h_n$, to accuracy *eps* is:

$h_0 := b_0$; if $(h_0 = 0)$ $h_0 :=$ small
$D_0 := 0$; $C_0 := h_0$
for $n = 1$, limit do begin
$D_n := b_n + a_n \cdot D_{n-1}$; if $(D_n = 0)$ $D_n :=$ small
$C_n := b_n + a_n / C_{n-1}$; if $(C_n = 0)$ $C_n :=$ small
$D_n := 1/D_n$
$\Delta_n := D_n \cdot C_n$; $h_n := h_{n-1} \Delta_n$
if $(|\Delta_n - 1| < eps)$ exit
end

Note. 1. The parameter *small* should be some non-zero number less than typical values of $eps \cdot |b_n|$, e.g., 10^{-50}.

2. It is necessary in a robust algorithm, as is also pointed out in [59], to monitor *both* the numerator and denominator ratios for approaches to zero. Our modification involves minimal change to the algorithm, whereas [59, (8)] proposes an altered recurrence relation after the denominator zero (in addition to Lentz's [58] treatment of numerator zeros).

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