Available online at www.sciencedirect.com
SCIENCE DIRECT®
Computer Physics Communications 159 (2004) 55–62
Computer Physics Communications
www.elsevier.com/locate/cpc

Evaluation of negative energy Coulomb (Whittaker) functions ☆

C.J. Noble

Computational Science and Engineering Department, CLRC Daresbury Laboratory, Warrington WA4 4AD, UK

Received 20 June 2001; accepted 9 December 2003

Abstract

This paper describes a code for evaluating exponentially decaying negative energy Coulomb functions and their first derivatives with respect to the radial variable. The functions, which correspond to Whittaker functions of the second kind, are obtained to high accuracy for a wide range of parameters using recurrence techniques.

Program summary

Title of program: whittaker_w
Catalog identifier: ADSZ
Program summary URL: http://cpc.cs.qub.ac.uk/summaries/ADSZ
Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland
Computer: Cray T3E, Sun Ultra-5_10 sparc, Origin2000, Compaq EV67, IBM SP3, Toshiba 460CDT
Operating systems under which the program has been tested: Windows NT4, Redhat Linux, SunOS 5.8
Programming language used: Fortran 95
Memory required to run with typical data: 500 KB
Number of bytes in distributed program, including test data, etc.: 39728
Number of lines in distributed program, including test data, etc.: 2900
Distribution format: tar gzip file
Nature of physical problem: The closed-channel components of the asymptotic radial wave function corresponding to electron or positron scattering by atomic or molecular ions may be expressed in terms of negative energy Coulomb functions. The scattering observables are obtained from S or T matrices which in turn are obtained by matching the radial and asymptotic wavefunctions at a finite radial point. Recent large scale scattering calculations have required accurate values of the Coulomb functions at smaller ρ values and larger negative η values than previous work. The present program is designed to extend the range of parameters for which the function may be calculated.
Method of solution: Recurrence relations, power series expansion, numerical quadrature.
Restrictions on the complexity of the problem: The program has been tested for the parameter ranges: $0 < \rho \leqslant 1000$, $|\eta| \leqslant 120$ and $0 \leqslant l \leqslant 100$. These ranges may, with appropriate scaling to avoid underflow and overflow, be extended.
References: A. Sunderland, C.J. Noble, P.G. Burke, V.M. Burke, Comp. Phys. Commun. 145 (2002) 311.

☆ This paper and its corresponding computer program are available via the Computer Physics Communications homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

E-mail address: c.j.noble@dl.ac.uk (C.J. Noble).

0010-4655/$ – see front matter
doi:10.1016/j.comphy.2003.12.004

Keywords: Negative energy; Coulomb; Whittaker; Confluent hypergeometric; Recurrence; Continued fraction; Matching; R-matrix

1. Introduction

Negative-energy Coulomb functions arise in a range of quantum mechanical scattering problems including nuclear, molecular and atomic collisions. A variety of methods have been used to evaluate these functions. Some of these techniques are able to provide very accurate values of the Coulomb functions. However, almost without exception, round-off error limits the range of parameters which may be treated. The present program is designed to provide accurate values of the exponentially decaying negative-energy coulomb function and its first derivative for a wider range of parameters than presently available programs. Real arguments are assumed but the program may be easily adapted to treat complex values.

Recently there has been progress in the development of computer programs based on R-matrix theory to treat electron scattering by atoms and atomic ions in the iron-peak region of the periodic table [1]. These targets are characterized by an open 3d electronic shell and exhibit a dense spectrum of states. As a consequence accurate scattering calculations employing a close-coupling expansion must typically include several hundred target states. The size of the computations generally means they must be carried out on powerful multi-processor computers. Further problems arise because of the dense energy-spacing of these target states. Traditionally this situation is treated either by taking near-degenerate targets as degenerate or by Gailitis averaging [2]. In the case of iron-peak targets both of these approaches introduce unacceptably large errors. This situation has stimulated the development of methods capable of obtaining accurate solutions of the scattering equations close to threshold.

R-matrix theory divides the collision into two or more regions and matches the logarithmic derivatives of the wavefunctions in adjacent regions. This matching, for example in the case of an ionic core, involves both positive and negative energy Coulomb functions. Close to target thresholds the matching requires exponentially decaying negative energy Coulomb functions for a wide range of parameters. This requirement motivates the development of the present program.

2. Theory

The negative-energy Coulomb functions satisfy a radial Schrödinger equation which may be written in scaled atomic units as

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{l(l+1)}{x^2} \pm \frac{2}{x} - \kappa^2\right) u_l(x) = 0, \tag{1}$$

where $x = Zr$ and the potential term is positive or negative for attractive and repulsive forces, respectively. The (positive) residual charge is denoted by Z and l is the orbital angular momentum. In the case of an electron or positron in the field of a nucleus of infinite mass the scattering energy, E, is given by

$$\frac{E}{Z^2} = -\frac{\kappa^2}{2} \tag{2}$$

for E in atomic units. On setting $\rho = \kappa x$, Eq. (1) takes the form

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} - \frac{l(l+1)}{\rho^2} - \frac{2\eta}{\rho} - 1\right) u_l(\rho) = 0. \tag{3}$$

The Coulomb parameter, η, is given by

$$\eta = \frac{\mp 1}{\kappa} \tag{4}$$

for attractive and repulsive forces, respectively.

The decaying solution may be expressed in terms of Whittaker functions (Abramowitz and Stegun, 1965, [4])[1] as

$$u_l(\eta;\rho) = W_{-\eta,l+1/2}(2\rho) \tag{5}$$

or alternatively in terms of the second confluent hypergeometric function, $U(a,c;x)$ as AS(13.1.33)

$$u_l(\eta;\rho) = \mathrm{e}^{-\rho}(2\rho)^{l+1} U(l+1+\eta, 2l+2, 2\rho). \tag{6}$$

The exponentially increasing Whittaker function, is related to the first confluent hypergeometric function, $M(a,c;x)$, AS(13.1.32). This is an entire function easily calculated from the expansion AS(13.1.2) (see,

[1] Equations from the NBS Handbook are referenced using the notation $AS(x.y.z)$.

for example, Neu and Shaw [3]). Normally this function is not required in the asymptotic matching of scattering wave functions and so will not be considered further here.

The properties of both positive and negative energy Coulomb functions have recently been reviewed by Seaton [5,6]. He has also published computer programs based on the use of series expansions [6] and a Numerov integration scheme [7]. The properties of the Whittaker and confluent hypergeometric functions have been detailed by Buchholz [8], Whittaker and Watson [9], Erdéyli et al. [10] and Slater [11]. Computer programs for calculating the negative energy Coulomb functions, or Whittaker functions of the second kind, have been developed for repulsive Coulomb forces by Hebbard and Robson [12]. Programs for treating attractive Coulomb forces have been developed by Bell and Scott [13] (using various expansions methods, including Chebyshev expansions and numerical integration) and by Noble and Thompson [14] using a series acceleration technique to analytically continue the asymptotic series representation of the Whittaker function. This latter method is robust and provides very accurate values of the functions for a wide range of parameters. A very similar approach using the Pade method to accelerate the asymptotic series representation has been proposed by Izarra et al. [15]. An efficient nonlinear sequence transformation for summing the divergent asymptotic series representation was subsequently proposed by Weniger [16]. The sequence transformation technique is particularly effective but eventually, like the technique of Noble and Thompson, is affected by roundoff errors for large negative values of η.

There exists a considerable body of research on methods for computing the confluent hypergeometric function of the second kind. Neumann series expansions have been derived by Badralexe et al. [17]. Algorithms for the rational approximation of confluent hypergeometric functions have been given by Luke [18]. Recurrence methods have also been developed which are particularly stable and easily specialized to calculate Coulomb functions. Methods based on extensions of the Miller technique form the basis of the present program.

Other approaches which have been considered and which may be effective in some circumstances include analytic continuation of the Frobenius expansion about the origin (Holubec and Stauffer [19]) and numerical integration of the differential equation. Seaton [7] has provided an efficient Numerov package and has emphasized the utility of such an approach at intermediate radial distances or whenever the functions are required for a range of radial variables. In the oscillatory region, the Whittaker function for large negative η values varies rapidly as a function of the radial variable ρ. In this situation the Numerov integration requires small step sizes and becomes less efficient. Extensions of the Numerov approach such as the exponentially fitted method described by Simos [20] are more effective in this situation and may be used to provide highly accurate values of the function.

3. Recurrence methods

Wimp [21] has shown that the hypergeometric function, $U(a,c;x)$, may be obtained by solving the three-term recurrence relation

$$\begin{aligned}&(n+a)(n+a+1-c)y(n)\\&\quad-(n+1)\big[2(n+a+1)+x-c\big]y(n+1)\\&\quad+(n+1)(n+2)y(n+2)=0.\end{aligned}\tag{7}$$

This second-order homogeneous difference equation has two linearly independent solutions. The required solution, $y(n)$, is termed *minimal* and any second solution, $v(n)$ is termed *dominant* provided

$$y(n)/v(n)\to 0,\quad \text{as } n\to\infty.\tag{8}$$

The minimal solution (if it exists) is unique and may be obtained by use of the Miller algorithm (Press et al. [22, p. 175]). First, an unnormalized solution, $y_N(n)$, is generated by downward recurrence from starting values

$$y_N(N)=1,\qquad y_{N+1}(N)=0.\tag{9}$$

The solution is then normalized using the convergent series (Wimp [21])

$$\sum_{n=0}^{\infty}y(n)=1,\qquad |\arg x|<\pi\tag{10}$$

derived from the integral representation (Erdéyli et al. [10, (3), p. 256]). Wimp also shows that $y(n)$ is related to the confluent hypergeometric function, $U(a,c,x)$,

by the equation

$$y(n) = \frac{x^a (a)_n (a+1-c)_n}{n!} U(a+n, c; x), \tag{11}$$

where $(a)_n$ represents Pochhammer's symbol *AS*(5.1.22). The method is stable and converges like

$$\mathrm{e}^{-\beta |x|^{1/2} n^{1/2}} \tag{12}$$

for some $\beta > 0$.

To avoid the necessity of repeating the calculation for several values of the integer N, an alternative algorithm for obtaining minimal solutions of three-term recurrence relations proposed by Gautschi [23] is employed. The algorithm is based on the use of the duality theorem due to Shintani [24] (see also Wimp [25]). The theorem states that the solution, $y_N(n)$, of a 3-term recurrence relation of the form

$$y(n) + a(n) y(n+1) + b(n) y(n+2) = 0 \tag{13}$$

satisfies the equation

$$b(N) y_N(n) + a(N+1) y_{N+1}(n) + y_{N+2}(n) = 0, \quad 0 \leqslant N = n, n+1, n+2, \ldots, \tag{14}$$

with initial conditions

$$y_n(n) = 1, \qquad y_{n+1}(n) = -a(n) \tag{15}$$

and

$$S_N(n) = \sum_{k=n}^{N} y_N(k) \tag{16}$$

satisfies

$$b(N) S_N(n) + a(N+1) S_{N+1}(n) + S_{N+2}(n) = 1, \quad 0 \leqslant N = n, n+1, \ldots, \tag{17}$$

with initial conditions

$$S_n(n) = 1, \qquad S_{n+1}(n) = -a(n) + 1. \tag{18}$$

The Gautschi algorithm avoids the necessity of repeated calculations when the starting value N is unknown. Moreover, by expressing the recurrence in the form of a continued fraction much of the scaling needed to keep the computed quantities within the range of the machine arithmetic can be avoided.

The ratio

$$r(n) = \frac{y(n+1)}{y(n)} \tag{19}$$

satisfies the relation

$$r(n) = \frac{-1}{a(n) + b(n) r(n+1)} \tag{20}$$

and is evaluated for some specified integer $n = K$. The forward evaluation of the resulting continued fraction is carried out in this program using the Lenz–Thompson algorithm [26]. Given $r(K)$ and $S(K)$ the solutions $y(1), y(2), \ldots, y(K)$ may be computed.

The Gautschi algorithm provides a very robust and rapid method for obtaining the confluent hypergeometric functions over most of the parameter range under consideration. However, as noted by Temme [27], the use of the Wimp recurrence relation Eq. (7) suffers from the accumulation of round-off errors at small values of x, particularly for large negative values of the parameter a. For the small x range Temme suggested downward recursion from computed $U(a+n, c, x)$ values. These starting values are obtained from asymptotic expressions for $a \to \infty$ involving sums of modified Bessel functions [28]. In the present program a simpler approach is adopted. It is noted that for values of the parameter a in the range $0 \leqslant a \leqslant 4$ the Gautschi method is accurate for $x \geqslant 0.8$. It is more convenient therefore to use this method to obtain the starting values for downward recurrence using continued fractions as in the Gautschi algorithm.

For values of $x \leqslant 0.8$ the U functions are computed using the power series about the origin given by *AS*(13.1.6). A sequence transformation [16] is applied to the expansion. This transformation does not extend the range of convergence of the expansion in the dramatic way seen when the same transformation is applied to an asymptotic expansion of the Whittaker function.

The methods described above are sufficient to obtain the U functions to at least 6–7 significant figures throughout the parameter space corresponding to $\eta \leqslant 0$ and $l = 0$. The approach is also accurate for a wide range of l values. In the present program if $l > 5$, corresponding to $c > 12$, the function is obtained by upward recurrence using the stable [27] relation *AS*(13.4.16). Values of the function derivatives with respect to x are obtained from the relation *AS*(13.4.21)

$$U'(a, c; x) = -a U(a+1, c+1 : x). \tag{21}$$

For positive values of a the Gautschi approach is accurate for values of $x \geqslant 12$ for the largest values of

a, c considered. For values of $\eta \geqslant 3$ and $0.8 < x < 12$ we obtain the functions from the integral representation *AS*(13.2.5) by numerical quadrature [12] using a Gauss–Laguerre formula. Quadrature weights and nodes are generated within the program using the LAPACK [29] routine *dstevx* to obtain the eigenvalues and eigenvectors of a tridiagonal matrix. This option allows the accuracy of the results to be adjusted easily. The surprising accuracy obtainable using the trapezoidal quadrature rule has been investigated by Allasia and Besenghi [30].

4. Program description

The routines are written in Fortran 95 and are contained in three modules, *whittaker_w*, *weniger* and *simos*. The third module, *simos*, is required only if the Coulomb differential equation is to be integrated to obtain function values at a sequence of radial points. The programs have been tested on a number of compilers for compliance with the f90 and f95 standards.

4.1. Coulomb–Whittaker functions

The principal routines of the package are contained within the f95 module *whittaker_w*. Three user-accessible routines are provided. The routine *coulomb_whittaker* has an argument list:

subroutine coulomb_whittaker $(\eta, l, \rho, w, wd, sf, err)$

The real variables η and ρ corresponding to the Coulomb parameter, Eq. (4), and the radial variable, ρ, are defined in Eq. (3). These, and the integer orbital angular momentum variable, l, must be provided as input. The real variable *err* is optional and sets the convergence threshold for the continued fraction evaluations. The default value is 1.0e–14 and under normal circumstance need not be changed.

The routine returns the negative energy Coulomb function, $u_l(\rho)$, as the real argument w and the value of its first derivative with respect to ρ as the real argument *wd*. The values are scaled by powers of 10 according to the returned value of the integer scale factor, *sf*.

Two subsidiary routines, *cw_force_method* and *cw_force_recur* allow the default choice of the computational method to be overridden. The computational method is defined by the module variable *method* which takes the values:

(1) Laguerre polynomial case, $U(-n, \alpha+1, x)$, for n a non-positive integer;
(2) finite polynomial case, $U(a, a+n+1, x)$, for n integral;
(3) transformed power series about the origin;
(4) numerical quadrature of the integral representation;
(5) Gautschi recurrence algorithm;
(6) modified Temme recurrence algorithm (downwards recurrence);
(7) Weniger transformed asymptotic series.

The default setting for the switch *method* is determined by the routine *select_method*. The choice is designed to guarantee as far as possible results of at least the minimum accuracy throughout the parameter space (limitations will be discussed in the following section). Computational times of Coulomb functions are not a significant factor in atomic scattering applications and so have not been taken into account in the construction of the driving routine. Nevertheless comparisons that we have carried out suggest that the principal calculational techniques which have been employed are competitive with alternative procedures. The Weniger option is included but not called by default. The selection algorithm which determines the computational method is illustrated diagrammatically in Fig. 1.

Calls to *cw_force_method* with an integer argument corresponding to one of the above methods will force subsequent calls to *coulomb_whittaker* to use that method exclusively. Similarly a call to *cw_force_recur* with a logical argument will force all subsequent calls to *coulomb_whittaker* to either always recur from $c = 2$ or to never use c-recursion.

There are several global variables used to control the scaling needed to avoid underflow and overflow. These are the variables *vbig*, *vsmall* and *small*. In ordinary circumstances these will not need to be changed. Two additional integer variables, *wp* and *fo* would normally be supplied from external modules and define the working precision kind value and the unit number for the output of error messages, respectively.

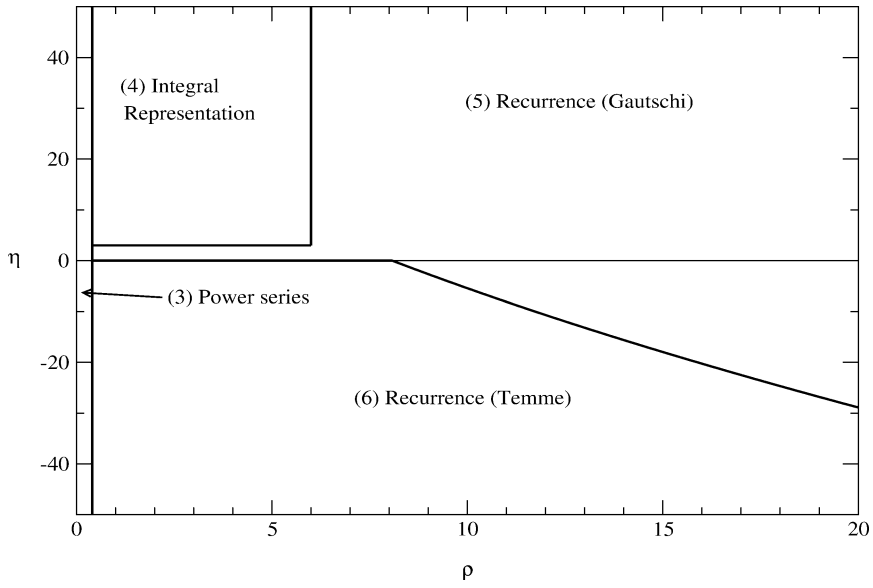

Fig. 1. Algorithm selection used in *whittaker_w*.

The procedures for performing the nonlinear sequence transformation defined by Weniger are defined in the module *weniger*. The single user-accessible routine in this module is the program *levin_weniger*. This has the calling sequence

subroutine levin_weniger (a, f, n, err).

Real argument a corresponds to an input array $a(0:n)$ of the first $n+1$ terms of the series to be summed using the sequence transformation. The estimated sum is returned as the second (real) argument f along with an estimate of the truncation error, *err*.

4.2. Numerical integration of the negative-energy Coulomb equation

The third module, *simos*, is provided for situations where the Coulomb functions are required for a sequence of radial values (for example in order to compute matrix elements). A very simple driver routine is provided to illustrate the use of the Simos integrator. Modifications will be necessary to perform production calculations, as for example provided in the Seaton code NUMER [7].

The integration method is required to integrate exactly any linear combination of the functions

$$x^i \sin(\phi x), \qquad x^i \cos(\phi x), \quad i = 0, \ldots, 3, \tag{22}$$

in the oscillatory region. A Numerov procedure is adequate in the exponential region but for convenience an exponentially fitted rule which integrates exactly the functions

$$x^i \exp(\pm v x), \quad i = 0, \ldots, 3, \tag{23}$$

is used. The parameters, ϕ and v are chosen using the approach of Ixaru and Rizea [31]. The large amplitude with which the functions may oscillate is illustrated in Fig. 2 which depicts $|u_l(\rho)|$ for the case $l = 0, \eta = -20.5$.

A detailed comparison of the Simos and Numerov approaches has not been attempted. A simple comparison using the same data as provided for the *simos* test run indicates that in many cases the Numerov results are accurate to only 2–3 significant figures. A comparison of the Simos approach with the results from the *coulomb_whittaker* routine indicates that the Simos integrator can provide very accurate values of the Coulomb–Whittaker function throughout the range of parameters considered here.

5. Testing and test run

The method selection is effectively determined by locating the radial values below which the Gautschi

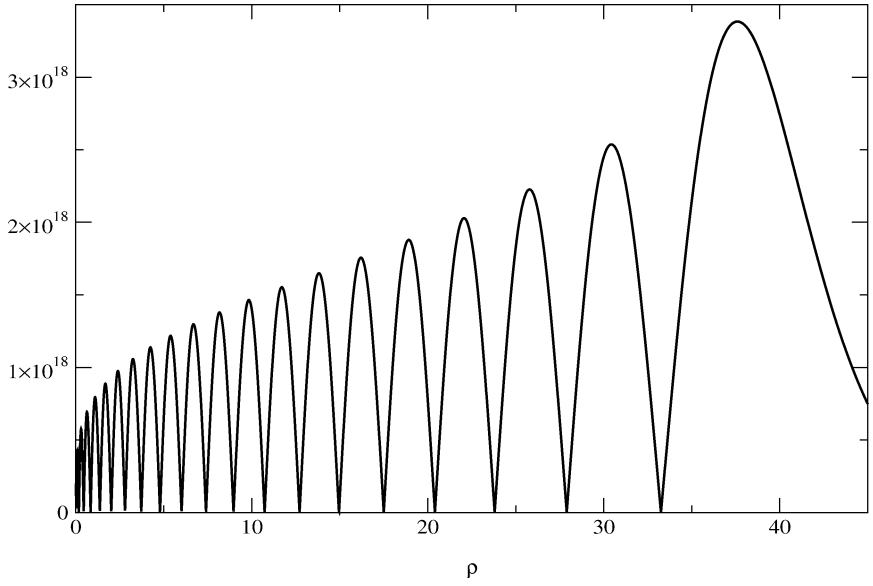

Fig. 2. Modulus of the Coulomb function $u_l(\rho)$ for $l = 0$ and $\eta = -20.5$.

recurrence approach is subject to significant roundoff error. These limits have been determined by comparing the results of calculations using double and extended (128-bit) precision. The results were fitted to a quadratic in the variable η. The quadratic fit is used to determine when the downward recurrence approach should be used.

The *coulomb_whittaker* code has been checked against a range of existing results and compared with results using extended precision. These indicate that results accurate to at least 7 significant figures are obtained apart from two regions. First for $\eta < 0$ and $0.5 \leqslant \rho \leqslant 1.5$ there are cases where only 4–5 significant figures are obtained. Second for $\eta \geqslant 70$ there is some loss of accuracy for $\rho \leqslant 0.4$. If greater accuracy is required in these regions either the Weniger (7) or the *simos* integration methods should be used. The present routine does not provide automatic switching to these alternative methods.

The main program, *whittaker_w_test.f*90, illustrates the use of the routine *coulomb_whittaker*. Sample input data in the file *testrun.dat* corresponds to representative values of the parameters in the range $0 \leqslant l \leqslant 100$, $0 < \rho \leqslant 100$ and $-100 \leqslant \eta \leqslant 100$. The output obtained on an IBM RS6000 is given in the file *test_run.out*. The second program, *simos_test.f*90, illustrates the use of the *simos* module. Here sample input and output is provided in the files *test_run*2.*dat* and *test_run*2.*out*.

References

[1] A. Sunderland, C.J. Noble, P.G. Burke, V.M. Burke, Comp. Phys. Commun. 145 (2002) 311.
[2] M. Gailitis, Zh. Eksp. Teor. Phys. 44 (1963) 1974, Sov. Phys. JETP 17 (1963) 1328.
[3] W.L. Neu, R.P. Shaw, Microsoftware for Engineers 2 (1986) 126.
[4] M. Abramowitz, I.A. Stegun, Handbook of Mathematical Functions, Dover, New York, 1965.
[5] M.J. Seaton, Comput. Phys. Commun. 146 (2002) 225.
[6] M.J. Seaton, Comput. Phys. Commun. 146 (2002) 250.
[7] M.J. Seaton, Comput. Phys. Commun. 146 (2002) 254.
[8] H. Buchholz, The Confluent Hypergeometric Function, Springer-Verlag, Berlin, 1969.
[9] E.T. Whittaker, G.N. Watson, A Course of Modern Analysis, Cambridge Univ. Press, Cambridge, 1963.
[10] A. Erdélyi, W. Magnus, F. Oberhettinger, F.G. Tricomi, Higher Transcendental Functions, vol. 1, McGraw–Hill, New York, 1953.
[11] L.J. Slater, Confluent Hypergeometric Functions, Cambridge Univ. Press, Cambridge, 1960.
[12] D.F. Hebbard, B.A. Robson, Nucl. Phys. 42 (1963) 563.
[13] K.L. Bell, N.S. Scott, Comput. Phys. Commun. 20 (1980) 447.
[14] C.J. Noble, I.J. Thompson, Comput. Phys. Commun. 33 (1984) 413.
[15] C. de Izarra, O. Vallée, J. Picart, N. Tran Minh, Comput. Phys. 9 (1995) 318.

[16] E.J. Weniger, Comput. Phys. 10 (1996) 496.
[17] E. Badralexe, P. Marksteiner, Y. Oli, A.J. Freeman, Comput. Phys. Commun. 71 (1992) 47.
[18] Y.L. Luke, Utilitas Math. 11 (1977) 123.
[19] A. Holubec, A.D. Stauffer, J. Phys. A: Math. Gen. 18 (1985) 2141.
[20] T.E. Simos, Helv. Phys. Acta 70 (1997) 781.
[21] J. Wimp, Computing 13 (1974) 195.
[22] W.H. Press, P.A. Teukolsky, W.T. Vetterling, B.R. Flannery, Numerical Recipes in FORTRAN, Cambridge Univ. Press, Cambridge, 1992.
[23] W. Gautschi, SIAM Rev. 9 (1967) 24.
[24] H. Shintani, J. Sci. Hiroshima Univ. 29 (1965) 121.
[25] J. Wimp, Computation with Recurrence Relations, Pitman, Boston, 1984.
[26] A.R. Barnett, in: K. Bartschat (Ed.), Computational Atomic Physics, Electron and Positron Collisions with Atoms and Ions, Springer-Verlag, Berlin, 1996.
[27] N.M. Temme, Num. Math. 41 (1983) 63.
[28] N.M. Temme, J. Comp. Appl. Math. 7 (1981) 27.
[29] E. Anderson, Z. Bai, C. Bischof, L.S. Blackford, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, D. Sorensen, LAPACK Users' Guide, third ed., SIAM, Philadelphia, 1999.
[30] G. Allasia, R. Besenghi, Computing 39 (1987) 271.
[31] L.G. Ixaru, M. Rizea, Comput. Phys. Commun. 19 (1980) 23.