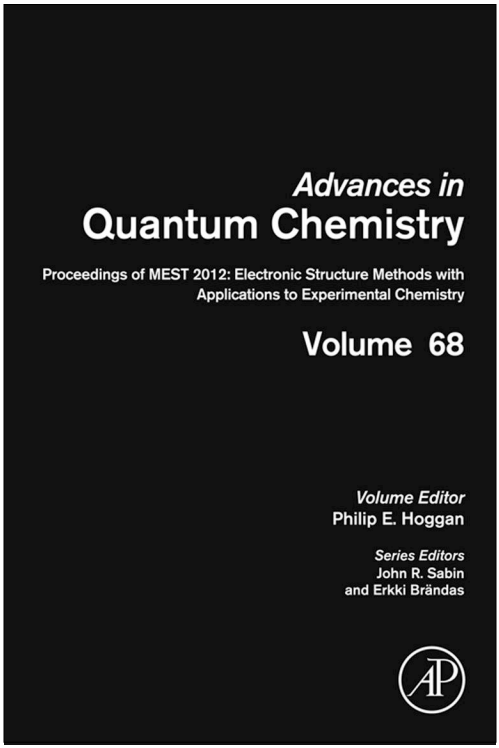

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CHAPTER THREE

Asymptotic Expansions of Barnett–Coulson–Löwdin Functions of High Order

A. Sidi[a], D. Pinchon[b] and P.E. Hoggan[c]

[a]Computer Science Department, Technion—Israel Institute of Technology, Haifa 32000, Israel
[b]Toulouse Institute of Mathematics, Université Paul Sabatier, 118 route de Narbonne, 31062 Toulouse Cedex, France
[c]LASMEA, UMR 6602 CNRS, Institut Pascal, LabEx IMobS3, 24 avenue des Landais, BP 80026, Aubiere Cedex 63170, France

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Abstract

The Barnett–Coulson–Löwdin functions (BCLFs) arise as coefficients in series expansions of Slater type orbitals about a displaced center. Following a detailed review of these functions, in this work, we provide full asymptotic expansions for them as the order of the modified Bessel functions that go into their construction tends to infinity. In doing so, we make use of some recent asymptotic expansions of modified Bessel functions that appeared in the paper [Ref. 22].

In molecular computations, BCLFs must be computed very many times. Therefore, it is necessary to design methods by which BCLFs can be computed efficiently. In this work, we also propose an iterative method for computing a whole sequence of BCLFs quickly, and accurately for some range of parameters. This method is implemented using quadruple-precision arithmetic, which is sufficient and present in some high-level programming language compilers used in scientific computing, such as FORTRAN 77 and C. The number of arithmetic operations needed for the proposed method is very small.

1. INTRODUCTION

The Barnett–Coulson–Löwdin functions (BCLFs) arise as coefficients in the series expansion of a Slater type orbital centered at a distance a from the origin, placed on an atomic nucleus where a set of Slater type orbitals are centered.[19,16] This allows the one- and two-electron multicenter integrals to be evaluated at a given origin in the molecule. The series expansion obtained is infinite, since the molecular geometry variable a (usually 1–20 a.u.) is fixed for an electronic structure calculation, whereas the instantaneous electron position variable r is independent of it and $0 < r < \infty$. They are both radial vectors and generally cannot be aligned.

The value of the screening parameter ζ generally exceeds 1 and should not exceed the atomic number. In practice, the lower limit for ζ is related to the first ionization potential I in atomic units, i.e., ζ must not be less than $\sqrt{2I}$. These limitations are helpful in establishing the numerical behavior of the BCLFs.

Much work is already available on BCLFs[12,13,17,14,15] and references therein. As is known, BCLFs are expressed in terms of the modified spherical Bessel functions $I_{n+1/2}(x)$ and $K_{n+1/2}(x)$, $n = 0, 1, \ldots$. In Section 2, we present an up-to-date review of the important properties of BCLFs known at present.

In Section 3, we derive the first known asymptotic expansions for BCLFs as the order of the modified Bessel functions used in their construction tends to infinity. These are based on some recent asymptotic expansions of Sidi and Hoggan[22] for the modified Bessel functions $I_\nu(z)$ and $K_\nu(z)$ as $\nu \to \infty$. We would like to emphasize that knowledge of these

expansions is helpful in deciding on what extrapolation method to use in order to accelerate the convergence of the infinite series mentioned in the first paragraph, which converge slowly. In Section 3, we also analyze the asymptotic behavior of BCLFs as the instantaneous electron position variable r tends to zero and to infinity.

In Section 4, we propose to compute a whole array of BCLFs simultaneously and quickly via one of the known recursion relations among the different BCLFs reviewed in Section 2. In Section 5, we discuss the algorithmic details of our method. It is important to note that, in this method, we do not compute $I_{n+1/2}(x)$ and $K_{n+1/2}(x)$ directly. Taking into account the asymptotics of $I_\nu(x)$ and $K_\nu(x)$ as $\nu \to \infty$, we compute some appropriately scaled versions of these functions instead. The scaling we use enables us to avoid the underflows and overflows that may occur in direct computation of $I_{n+1/2}(x)$ and $K_{n+1/2}(x)$ for large values of n; it is thus an important ingredient of our method. This also allows us to scale the BCLFs appropriately. In order to end up with BCLFs that have double-precision accuracy, in our method, we compute both the functions $I_{n+1/2}(x)$ and $K_{n+1/2}(x)$ and the BCLFs in quadruple-precision arithmetic, the idea being that the quadruple-precision arithmetic is shown to suffice and it is offered with some high-level programming language compilers used for scientific applications, such as Fortran 77 and C. As the number of arithmetic operations required is very small (of the order of wN, where N is the number of BCLFs computed and w is a small integer), the use of quadruple-precision arithmetic cannot increase the cost of the computation timewise.

In Appendix A, we summarize the results of [22] that are relevant to the present work. In Appendix B, we discuss the recursive computation of the scaled versions of $I_{n+1/2}(x)$ and $K_{m+1/2}(x)$ that avoids overflows and underflows in floating-point arithmetic. In Appendix C, we show that the recursive computation of the scaled versions of $I_{n+1/2}(x)$ (backward) and $K_{m+1/2}(x)$ (forward) is stable numerically.

2. REVIEW OF BCLFs

2.1 Definition and properties of BCLFs

Let n be a non-negative integer, and let a,r, and ζ be as described in the first and second paragraphs of the Introduction. Thus, a and ζ are finite, while r assumes values from 0 to infinity. With R defined as in

$$R = \sqrt{a^2 + r^2 - 2ar\cos\theta} \tag{1}$$

consider the function $R^{n-1}e^{-\zeta R}$. Letting $x = \cos\theta$ so that $x \in [-1, +1]$, its expansion in Legendre polynomials $P_\lambda(x)$ may be expressed as

$$R^{n-1}e^{-\zeta R} = \frac{1}{\sqrt{ar}} \sum_{\lambda=0}^{\infty} (2\lambda+1) A^n_{\lambda+1/2}(\zeta, a, r)\, P_\lambda(x), \quad -1 \le x \le 1, \tag{2}$$

$A^n_{\lambda+1/2}$ being the BCLFs. From this relation, it is seen that $R^{n-1}e^{-\zeta R}$ serves as a "generating function" for the BCLFs. Since

$$\int_{-1}^{+1} P^2_\lambda(x)\, dx = \frac{2}{2\lambda+1}, \quad \lambda = 0, 1, \ldots, \tag{3}$$

we immediately deduce from (2) that

$$A^n_{\lambda+1/2}(\zeta, a, r) = \frac{\sqrt{ar}}{2} \int_{-1}^{+1} R^{n-1}e^{-\zeta R} P_\lambda(x)\, dx, \quad \lambda = 0, 1, \ldots \tag{4}$$

Clearly, the $A^n_{\lambda+1/2}(\zeta, a, r)$ are symmetric functions of a and r, that is,

$$A^n_{\lambda+1/2}(\zeta, a, r) = A^n_{\lambda+1/2}(\zeta, r, a), \tag{5}$$

because the function $R^{n-1}e^{-\zeta R}$ is.

A simple expression for BCLFs with $n = 0$ and $\lambda = 0, 1, \ldots$, is known (see Abramowitz and Stegun Ref. 1, p. 445, formula 10.2.35):

$$A^0_{\lambda+1/2}(\zeta, a, r) = I_{\lambda+1/2}(\zeta\rho) K_{\lambda+1/2}(\zeta\rho'); \quad \rho = \min\{a, r\}, \quad \rho' = \max\{a, r\}. \tag{6}$$

Here, $I_{\lambda+1/2}(x)$ and $K_{\lambda+1/2}(x)$ are the modified spherical Bessel functions[1] of order λ, of the first and third kind, respectively. Because $I_{\lambda+1/2}(x)$ and $K_{\lambda+1/2}(x)$ are defined for *all* integer values of λ, we let (6) *define* $A^0_{\lambda+1/2}(\zeta, a, r)$ for $\lambda < 0$ as well. This is an important step that enables us to *define* $A^n_{\lambda+1/2}(\zeta, a, r)$ for $\lambda < 0$ as well, which is what we consider next.

From the integral representation in (4), it follows that, for $n \ge 0$,

[1] The functions $I_{\lambda+1/2}(x)$ and $K_{\lambda+1/2}(x)$ satisfy three-term recursion relations in λ that are given in (65) and (66) in this work, and are defined for *all* integer values of λ. Those $I_{\lambda+1/2}(x)$ with $\lambda \ge 0$ are called modified spherical Bessel functions of the first kind, while those with $\lambda < 0$ are called modified spherical Bessel functions of the second kind. The $K_{\lambda+1/2}(x)$ are called modified spherical Bessel functions of the third kind. Each of the two pairs $[I_{\lambda+1/2}(x)$ and $I_{-\lambda-1/2}(x)]$ and $[I_{\lambda+1/2}(x)$ and $K_{\lambda+1/2}(x)]$ is a linearly independent set of solutions of the modified spherical Bessel equation of order λ. See Abramowitz and Stegun [Ref. 1, Chapter 10].

$$A^{n+1}_{\lambda+1/2}(\zeta, a, r) = -\frac{\partial}{\partial \zeta} A^{n}_{\lambda+1/2}(\zeta, a, r), \tag{7}$$

and hence

$$A^{n}_{\lambda+1/2}(\zeta, a, r) = (-1)^{n} \frac{\partial^{n}}{\partial \zeta^{n}} A^{0}_{\lambda+1/2}(\zeta, a, r). \tag{8}$$

From (6), it is obvious that $A^{0}_{\lambda+1/2}(\zeta, a, r) = A^{0}_{\lambda+1/2}(1, \zeta a, \zeta r)$. By a simple manipulation of the integral representation in (4), it can be shown analogously that $A^{n}_{\lambda+1/2}(\zeta, a, r)$ satisfy the "homogeneity relation"

$$A^{n}_{\lambda+1/2}(\zeta, a, r) = \zeta^{-n} A^{n}_{\lambda+1/2}(1, \zeta a, \zeta r), \quad n \geq 0. \tag{9}$$

This relation shows that $A^{n}_{\lambda+1/2}(\zeta, a, r)$ are actually functions of two variables, namely, of ζa and ζr, and can be computed directly from the functions $\bar{A}^{n}_{\lambda}(a, r)$ that are defined as in

$$\bar{A}^{n}_{\lambda}(a, r) = A^{n}_{\lambda+1/2}(1, a, r). \tag{10}$$

From (9) and (10), it follows that $A^{n}_{\lambda+1/2}(\zeta, a, r)$ can be computed from $\bar{A}^{n}_{\lambda}(a, r)$ via

$$A^{n}_{\lambda+1/2}(\zeta, a, r) = \zeta^{-n} \bar{A}^{n}_{\lambda}(\zeta a, \zeta r). \tag{11}$$

Invoking (11), it is easy to show that (7) can be rewritten as

$$\bar{A}^{n+1}_{\lambda}(a, r) = n\bar{A}^{n}_{\lambda}(a, r) - \left(a\frac{\partial}{\partial a} + r\frac{\partial}{\partial r}\right) \bar{A}^{n}_{\lambda}(a, r), \quad n \geq 0. \tag{12}$$

2.2 Recurrence relations

Now, just as the $A^{0}_{\lambda+1/2}$ are defined for *all* integer values of λ, the $A^{n}_{\lambda+1/2}$, $n = 1, 2, \ldots$, too can be defined for *all* integer values of λ, and satisfy the following recurrence relations that are proved in Barnett[5]:

$$A^{1}_{\lambda+1/2}(\zeta, a, r) = \frac{ar\zeta}{2\lambda+1}\left[A^{0}_{\lambda-1/2}(\zeta, a, r) - A^{0}_{\lambda+3/2}(\zeta, a, r)\right] \tag{13}$$

and

$$A^{n+2}_{\lambda+1/2}(\zeta,a,r) = (a^2+r^2)A^n_{\lambda+1/2}(\zeta,a,r) - \frac{2ar}{2\lambda+1}\left[\lambda A^n_{\lambda-1/2}(\zeta,a,r) + (\lambda+1)A^n_{\lambda+3/2}(\zeta,a,r)\right]. \tag{14}$$

Of these, (13) can be obtained by first letting $n=0$ in (7) and invoking (6), and next employing the recursion relations among the $I_{\lambda+1/2}(x)$ and $K_{\lambda+1/2}(x)$ and their derivatives, which are valid for all integer values of λ. The relation in (14), with $\lambda \geq 0$, can be obtained by first replacing n by $n+2$ in (4), then writing $R^{n+1} = R^{n-1}R^2 = R^{n-1}(a^2+r^2-2arx)$, and then using the recursion relation among the Legendre polynomials to express $xP_\lambda(x)$ as a linear combination of $P_{\lambda-1}(x)$, $P_\lambda(x)$, and $P_{\lambda+1}(x)$, and finally, by invoking (4). Clearly, whenever $A^n_{\lambda+3/2}(\zeta,a,r)$ are defined for all integer values of λ, so are $A^{n+2}_{\lambda+1/2}(\zeta,a,r)$. From this, it follows that, because $A^0_{\lambda+3/2}(\zeta,a,r)$ are defined by (6) for all λ, so are $A^n_{\lambda+3/2}(\zeta,a,r)$ with $n=1,2,\ldots$, by (13) and (14).

Letting $\zeta = 1$ in (13) and (14), we obtain the equivalent recurrence relations

$$\bar{A}^1_\lambda(a,r) = \frac{ar}{2\lambda+1}\left[\bar{A}^0_{\lambda-1}(a,r) - \bar{A}^0_{\lambda+1}(a,r)\right] \tag{15}$$

$$\bar{A}^{n+2}_\lambda(a,r) = (a^2+r^2)\bar{A}^n_\lambda(a,r) - \frac{2ar}{2\lambda+1}\left[\lambda\bar{A}^n_{\lambda-1}(a,r) + (\lambda+1)\bar{A}^n_{\lambda+1}(a,r)\right], \quad n \geq 0. \tag{16}$$

Of course, the initial conditions are

$$\bar{A}^0_\lambda(a,r) = I_{\lambda+1/2}(\rho)K_{\lambda+1/2}(\rho'); \quad \rho = \min\{a,r\}, \quad \rho' = \max\{a,r\}. \tag{17}$$

Next, using (15) and (16), it is easily seen that $\bar{A}^n_\lambda(a,r)$ can be expressed as a linear combination of $\bar{A}^0_k$ as in

$$\bar{A}^n_\lambda(a,r) = \sum_{i=-\lfloor (n+1)/2\rfloor}^{\lfloor (n+1)/2\rfloor} p_{n,i}(a,r,\lambda)\bar{A}^0_{\lambda+i}(a,r). \tag{18}$$

Here, the $p_{n,i}(a,r,\lambda)$ are polynomial in a,r and rational in λ.

Remark. The following recurrence relation that appears in Bouferguène[6] is incorrect because it violates the homogeneity relation given in (9):

$$A_l^{n+1}(\zeta, a, r) = \frac{ar}{2l+1}\Big[A_{\lambda-1/2}^{n}(\zeta, a, r) - A_{\lambda+3/2}^{n}(\zeta, a, r) - A_{\lambda-1/2}^{n-1}(\zeta, a, r) - A_{\lambda+3/2}^{n-1}(\zeta, a, r)\Big].$$

2.3 Explicit expressions

The relations in (6) and (7), together with recurrence and derivative relations on Bessel functions, allow us to obtain explicit expressions for $A_{\lambda+1/2}^{n}(\zeta, a, r)$ in terms of the modified spherical Bessel functions for any n, λ, a, and r. For example, for $A_{\lambda+1/2}^{1}(\zeta, a, r)$, we have

$$A_{\lambda+1/2}^{1}(\zeta, a, r) = aI_{\lambda+1/2}(\zeta r)K_{\lambda-1/2}(\zeta a) - rI_{\lambda+3/2}(\zeta r)K_{\lambda+1/2}(\zeta a), \quad 0 \le r \le a, \tag{19}$$

$$A_{\lambda+1/2}^{1}(\zeta, a, r) = \frac{2\lambda+1}{\zeta}I_{\lambda+1/2}(\zeta r)K_{\lambda+1/2}(\zeta a) - rI_{\lambda-1/2}(\zeta r)K_{\lambda+1/2}(\zeta a) + aI_{\lambda+1/2}(\zeta r)K_{\lambda-1/2}(\zeta a), \quad 0 \le r \le a, \tag{20}$$

$$A_{\lambda+1/2}^{1}(\zeta, a, r) = -\frac{2\lambda+1}{\zeta}I_{\lambda+1/2}(\zeta r)K_{\lambda+1/2}(\zeta a) - rI_{\lambda+3/2}(\zeta r)K_{\lambda+1/2}(\zeta a) + aI_{\lambda+1/2}(\zeta r)K_{\lambda+3/2}(\zeta a), \quad 0 \le r \le a. \tag{21}$$

An explicit expression for $A_{\lambda}^{2}(a, r)$ that is analogous to that in (19) is

$$A_{\lambda}^{2}(a, r) = [a^2 + r^2 + 2\lambda(2\lambda+1)]I_{\lambda+1/2}(r)K_{\lambda+1/2}(a) + 2rI_{\lambda+3/2}(r)K_{\lambda+1/2}(a) - 2a\left[rI_{\lambda+3/2}(r)K_{\lambda+3/2}(a) + \lambda I_{\lambda+1/2}(r)K_{\lambda+3/2}(a)\right], \quad 0 \le r \le a. \tag{22}$$

We now turn to other expressions for BCLFs. Let us define a set of polynomials $p_n(x)$, $n \ge 0$, by the recurrence relation

$$p_n(x) = (2n-1)p_{n-1}(x) + x^2 p_{n-2}(x), \quad n \ge 2; \qquad p_0(x) = 1, \quad p_1(x) = x + 1. \tag{23}$$

Obviously, $p_n(x)$ have integer coefficients. For example,

$$p_2(x) = x^2 + 3x + 3, \quad p_3(x) = x^3 + 6x^2 + 15x + 15.$$

The polynomials $p_n(x)$ are encountered in Padé approximants of the function $f(x) = e^{2x}$, in the sense that

$$f_{n,n}(x) = \frac{p_n(x)}{p_n(-x)}, \quad n \geq 1, \tag{24}$$

is the $[n/n]$ Padé approximant[2] to $f(x) = e^{2x}$.

For n a non-negative integer, the functions $I_{n+1/2}(x)$ and $K_{n+1/2}(x)$ can be expressed in terms of the polynomial $p_n(x)$:

$$I_{n+1/2}(x) = (-1)^n \frac{x^{n+1/2}}{\sqrt{2\pi}} \left[\frac{p_n(-x)e^x - p_n(x)e^{-x}}{x^{2n+1}} \right], \tag{25}$$

the term inside the square brackets being a regular function at $x = 0$ with even parity,

$$K_{n+1/2}(x) = \frac{\sqrt{\pi}\, e^{-x}}{\sqrt{2}\, x^{n+1/2}}\, p_n(x). \tag{26}$$

Theorem 2.1 *The functions $\bar{A}^n_\lambda(a, r)$ have the following explicit representation:*

$$\bar{A}^n_\lambda(a, r) = \frac{e^{-a}}{2a^{\lambda+1/2} r^{\lambda+1/2}} \left[p^{(n)}_\lambda(a, r)e^r + q^{(n)}_\lambda(a, r)e^{-r} \right], \tag{27}$$

where $p^{(n)}_\lambda(a, r)$ and $q^{(n)}_\lambda(a, r)$ are polynomials in a and r with integer coefficients, with degree $n + \lambda$ with respect to each variable a, r and with total degree $n + 2\lambda$ with respect to a and r.

[2] $f_{m,n}(x) = \hat{p}(x)/\hat{q}(x)$ is the $[m/n]$ Padé approximant to a function $f(x)$, where $\hat{p}(x)$ and $\hat{q}(x)$ are relatively prime polynomials with respective degrees at most m and n and $\hat{q}(0) \neq 0$, such that $f(x) - \hat{p}(x)/\hat{q}(x) = O(x^{m+n+1})$ as $x \to 0$. Furthermore, when it exists, $f_{m,n}(x)$ is unique. For Padé approximants, see, for example, Baker and Graves–Morris[4] and Sidi [Ref. 20, Chapter 17].

2.4 Integral representations

As in Bouferguène and Rinaldi,[8] using the integral representation of the product of two modified Bessel functions (see Gradshteyn and Rhyzik Ref. 10, p. 703, Eq. (6.541)), we have

$$K_\nu(\zeta a)I_\nu(\zeta r) = \int_0^{+\infty} \frac{t}{t^2+\zeta^2} J_\nu(at)J_\nu(rt)\,dt, \quad 0 \le r \le a. \tag{28}$$

From (6) and (8), we then have

$$A^n_{\lambda+1/2}(\zeta, a, r) = \int_0^{+\infty} (-1)^n \frac{\partial^n}{\partial \zeta^n}\left(\frac{t}{t^2+\zeta^2}\right) J_{\lambda+1/2}(at)J_{\lambda+1/2}(rt)\,dt. \tag{29}$$

This is equivalent to Eq. (29) in Bouferguène and Rinaldi.[8]

The following integral representations are used in Ref.6:

$$A^0_{\lambda+1/2}(\zeta, a, r) = \frac{1}{2}\int_0^{+\infty} I_{\lambda+1/2}\left(\frac{ar}{2u}\right) \exp\left[-\zeta^2 u - \frac{a^2+r^2}{4u}\right]\frac{du}{u}, \tag{30}$$

$$A^n_{\lambda+1/2}(\zeta, a, r) = \frac{1}{2}\int_0^{+\infty} u^{n/2} H_n(\zeta\sqrt{u}) I_{\lambda+1/2}\left(\frac{ar}{2u}\right) \exp\left[-\zeta^2 u - \frac{a^2+r^2}{4u}\right]\frac{du}{u}, \tag{31}$$

where $H_n(x)$ is the Hermite polynomial of degree n.

2.5 BCLFs for $r=a$

Some simplifications take place in the recursion relations satisfied by BCLFs along the "diagonal" $r = a$. For integers $n \ge 1$ and $\lambda \ge 0$, define the functions $g^{(n)}_\lambda$ by

$$g^{(n)}_\lambda(a) = A^{(n)}_{\lambda+1/2}(1, a, a) = \bar{A}^{(n)}_\lambda(a, a). \tag{32}$$

It is straightforward to verify the following relations:

$$g^{(0)}_\lambda(a) = I_{\lambda+1/2}(a)K_{\lambda+1/2}(a), \tag{33}$$

$$g_\lambda^{(1)}(a) = \frac{a^2}{2\lambda+1}\left[g_{\lambda-1}^{(0)}(a) - g_{\lambda+1}^{(0)}(a)\right], \tag{34}$$

$$g_\lambda^{(n+1)}(a) = n g_\lambda^{(n)}(a) - a\frac{d}{da}g_\lambda^{(n)}(a), \quad n \geq 0, \tag{35}$$

$$g_\lambda^{(n+2)}(a) = 2a^2\left\{g_\lambda^{(n)}(a) - \frac{1}{2\lambda+1}\left[\lambda g_{\lambda-1}^{(n)}(a) + (\lambda+1)g_{\lambda+1}^{(n)}(a)\right]\right\}, \quad n \geq 0. \tag{36}$$

3. ASYMPTOTICS OF BCLFs

In this section, we study the asymptotic behavior of $\bar{A}_\lambda^n(a,r)$ (i) as $\lambda \to \infty$ while r is fixed and (ii) as $r \to 0$ and $r \to \infty$ while λ is fixed.

3.1 Asymptotics as $\lambda \to \infty$

When studying the asymptotics as $\lambda \to \infty$, we make use of the results of Appendix A as well as of those in Section 2. As the conclusions for $r \neq a$ and $r = a$ are different, we treat these two cases separately.

We begin with the case $r \neq a$.

Theorem 3.1 *Let $r \neq a$, and define $\rho = \min\{a, r\}$, $\rho' = \max\{a, r\}$, and $\sigma = \rho/\rho'$. Let also $\nu = \lambda + 1/2$ for simplicity of notation. Then*

$$\bar{A}_\lambda^n(a,r) \sim \frac{\sigma^\nu}{\nu}\sum_{s=s_n}^{\infty}\frac{w_{n,s}(a,r)}{\nu^s} \quad \text{as } \lambda \to \infty; \quad s_n = \left\lfloor \frac{n+1}{2} \right\rfloor, \tag{37}$$

where

$$w_{n,s_n}(a,r) = (-1)^{n+s_n}\frac{(2s_n)!}{2^{2s_n+1}s_n!}(\rho'^2 - \rho^2)^{s_n}, \quad n = 0, 1, \ldots \tag{38}$$

By the fact that $w_{n,s_n}(a,r) \neq 0$ when $r \neq a$, we also have the asymptotic equalities

$$\bar{A}_\lambda^n(a,r) \sim w_{n,s_n}(a,r)\frac{\sigma^\nu}{\nu^{s_n+1}} \quad \text{as } \lambda \to \infty, \quad n = 0, 1, \ldots \tag{39}$$

The nature of the $w_{n,s}(a,r)$ will be clear in the proof.

Remark. In particular, as $\lambda \to \infty$,

$$\bar{A}^0_\lambda(a,r) \sim \frac{1}{2}\frac{\sigma^\nu}{\nu}, \quad \bar{A}^1_\lambda(a,r) \sim \frac{\rho'^2-\rho^2}{4}\frac{\sigma^\nu}{\nu^2},$$
$$\bar{A}^2_\lambda(a,r) \sim -\frac{\rho'^2-\rho^2}{4}\frac{\sigma^\nu}{\nu^2}, \quad \text{and so on.} \tag{40}$$

Proof. We start with $n=0$. Let $r<a$ for simplicity of notation. Then, by (8), (6), and Theorem A.1, we have

$$\begin{aligned}\bar{A}^0_\lambda(\zeta a,\zeta r) &= A^0_\nu(\zeta,a,r)\\ &= I_\nu(\zeta r)K_\nu(\zeta a) \sim \frac{1}{2\nu}\left(\frac{r}{a}\right)^\nu \sum_{s=0}^{\infty}\frac{d_s(\zeta a,\zeta r)}{\nu^s} \quad \text{as } \lambda\to\infty,\end{aligned} \tag{41}$$

where

$$d_s(\zeta a,\zeta r) = \sum_{j=0}^{s}(-1)^{s-j}b_{s-j}(\zeta a)\,b_j(\zeta r), \quad s=0,1,\ldots, \tag{42}$$

$b_s(z)$ being a polynomial of degree s in z^2. Therefore, $d_s(\zeta a,\zeta r)$ is a polynomial of degree s in ζ^2, which we write as in

$$d_s(\zeta a,\zeta r) = \sum_{i=0}^{s}\gamma_{s,i}(a,r)\zeta^{2i}. \tag{43}$$

Note that, by (A.4) and (A.6), we have

$$\gamma_{s,s}(a,r) = \frac{1}{s!}\frac{a^{2s}}{4^s}\sum_{j=0}^{s}(-1)^{s-j}\binom{s}{j}\left(\frac{r^2}{a^2}\right)^j = \frac{(r^2-a^2)^s}{4^s s!} \neq 0. \tag{44}$$

We next consider the case $n\geq 1$. For this, we employ (8). Differentiating the asymptotic expansion in (41) with respect to ζ, we have

$$A^n_\nu(\zeta,a,r) \sim (-1)^n\frac{1}{2\nu}\left(\frac{r}{a}\right)^\nu\sum_{s=0}^{\infty}\frac{\frac{\partial^n}{\partial\zeta^n}d_s(\zeta a,\zeta r)}{\nu^s} \quad \text{as } \lambda\to\infty. \tag{45}$$

Because $d_s(\zeta a, \zeta r)$ is an even polynomial in ζ of degree $2s$, it follows that

$$\frac{\partial^n}{\partial \zeta^n} d_s(\zeta a, \zeta r) = 0 \quad \text{if } 2s < n. \tag{46}$$

By $s_n = \lfloor (n+1)/2 \rfloor$, we have that $2s < n$ implies $s < s_n$ when s is a nonnegative integer. Thus,

$$\frac{\partial^n}{\partial \zeta^n} d_s(\zeta a, \zeta r) = 0 \quad \text{if } s < s_n. \tag{47}$$

Therefore, by the fact that $\gamma_{s,s}(a, r) \neq 0$ for all s, the first nonzero term of the infinite sum in (45) is that with $s = s_n$, which is given by

$$\frac{\partial^n}{\partial \zeta^n} d_{s_n}(\zeta a, \zeta r) = \begin{cases} \gamma_{s_n,s_n}(a, r)\,(2s_n)!\,\zeta & \text{if } n = 2s_n - 1, \\ \gamma_{s_n,s_n}(a, r)\,(2s_n)! & \text{if } n = 2s_n, \end{cases} \tag{48}$$

so that

$$\frac{\partial^n}{\partial \zeta^n} d_{s_n}(\zeta a, \zeta r)\big|_{\zeta=1} = \gamma_{s_n,s_n}(a, r)\,(2s_n)! \quad \text{for all } n. \tag{49}$$

The results in (37) and (38) follow by combining (44), (47), (48), and (49) in (45), and letting $\zeta = 1$ there. Note also that $w_{n,s}(a, r) = (-1)^n \frac{\partial^n}{\partial \zeta^n} d_{s_n}(\zeta a, \zeta r)\big|_{\zeta=1}$. □

Remark. The asymptotic expansions given in (37) [but not (38)] can also be derived by using the recursion relations in (13) and (14).

We now consider the case $r = a$.

Theorem 3.2 *For fixed $a > 0$, and with $\nu = \lambda + 1/2$ as in Theorem 3.1, $\bar{A}^0_\lambda(a, a)$ has the asymptotic expansion*

$$\bar{A}^0_\lambda(a, a) \sim \frac{1}{2\nu} \sum_{s=0}^{\infty} \frac{p_s(a)}{\nu^{2s}} \quad \text{as } \lambda \to \infty, \tag{50}$$

where $p_s(a)$ are the polynomials defined in Theorem A.2; thus, $p_0(a) = 1$ and, for each $s = 1, 2, \ldots, p_s(a)$ is a polynomial of degree s in a^2 and $(-1)^s p_s(a)$ has non-negative coefficients. The leading coefficient u_s of $p_s(a)$ is given by

$$u_s = (-1)^s \frac{(2s-1)!!}{2^s s!}. \tag{51}$$

For $n \geq 1$ and fixed $a > 0$, $\bar{A}^n_\lambda(a, a)$ has the asymptotic expansion

$$\bar{A}^n_\lambda(a,a) \sim \frac{(-1)^n}{2\nu} \sum_{s=s_n}^{\infty} \frac{\partial^n}{\partial \zeta^n} p_s(\zeta a)\bigg|_{\zeta=1} \frac{1}{\nu^{2s}} \quad \text{as } \nu \to \infty; \quad s_n = \left\lfloor \frac{n+1}{2} \right\rfloor, \tag{52}$$

where $p_s(z)$ are exactly as before. Therefore, the following asymptotic equality is also valid:

$$\bar{A}^n_\lambda(a,a) \sim (-1)^{n+s_n} \frac{[(2s_n-1)!!]^2}{2} \frac{a^{2s_n}}{\nu^{2s_n+1}}, \quad \text{as } \lambda \to \infty. \tag{53}$$

Proof. The first part of the theorem pertaining to $\bar{A}^0_\lambda(a, a)$ follows from the fact that $\bar{A}^0_\lambda(a, a) = I_\nu(a)K_\nu(a)$ and from Theorem A.2.

By (10) and (7), the asymptotic expansion of $\bar{A}^n_\lambda(a, a)$ is given as in

$$\begin{aligned} \bar{A}^n_\lambda(a,a) &= \frac{(-1)^n}{2\nu} \frac{\partial^n}{\partial \zeta^n} \bar{A}^0_\lambda(\zeta a, \zeta a)\bigg|_{\zeta=1} \\ &\sim \frac{(-1)^n}{2\nu} \sum_{s=0}^{\infty} \frac{\partial^n}{\partial \zeta^n} p_s(\zeta a)\bigg|_{\zeta=1} \frac{1}{\nu^{2s}} \quad \text{as } \nu \to \infty. \end{aligned} \tag{54}$$

Because $p_s(\zeta a)$ is an even polynomial of degree $2s$ in ζ, it follows that

$$\frac{\partial^n}{\partial \zeta^n} p_s(\zeta a) = 0 \quad \text{if } 2s < n.$$

Thus, the infinite sum in (54) begins with the $s = s_n$ term. Furthermore, if $n = 2s - 1$ or $n = 2s$, then

$$\left.\frac{\partial^n}{\partial\zeta^n}p_s(\zeta\, a)\right|_{\zeta=1} = \frac{(-1)^n}{2}(2s)!\; u_s\; a^{2s} = (-1)^{n+s}\;\frac{[(2s_n-1)!!]^2}{2}a^{2s}. \tag{55}$$

This completes the proof. □

Note that the explicit expression for $p_s(a)$ given in Theorem A.2 and Eq. (54) allow an explicit expression for the asymptotic expansion $\bar{A}^n_\lambda(a,a)$ to be written. We leave the details to the reader.

3.2 Asymptotics as $r \to 0$ and $r \to \infty$

Because r ranges from zero to infinity, it is appropriate to analyze the behavior of the BCLFs as $r \to 0$ and as $r \to \infty$. For this, we need the following known asymptotic equalities that can be differentiated indefinitely:

$$I_\nu(x) \sim \frac{(x/2)^\nu}{\Gamma(\nu+1)} \quad \text{as } x \to 0, \qquad K_\nu(x) \sim \sqrt{\frac{\pi}{2x}}\, e^{-x} \quad \text{as } x \to \infty. \tag{56}$$

Theorem 3.3 *With λ fixed, the BCLFs satisfy the asymptotic equalities*

$$\bar{A}^n_\lambda(a,r) \sim D_{n,\lambda}\, r^{\lambda+1/2} \quad \text{as } r \to 0, \tag{57}$$

and

$$\bar{A}^n_\lambda(a,r) \sim E_{n,\lambda}\, r^{n-1/2} e^{-r} \quad \text{as } r \to \infty, \tag{58}$$

where $D_{n,\lambda}$ *and* $E_{n,\lambda}$ *are constants given as in*

$$D_{n,\lambda} = \frac{(-1)^n}{2^\nu\Gamma(\nu+1)}\sum_{i=0}^{n}\binom{n}{i}\left[\prod_{j=1}^{n-i}(\nu-j+1)\right]a^i K_\nu^{(i)}(a), \qquad \nu = \lambda+1/2, \tag{59}$$

and

$$E_{n,\lambda} = \sqrt{\frac{\pi}{2}}\, I_\nu(a), \qquad \nu = \lambda+1/2. \tag{60}$$

Proof. Letting $\nu = \lambda + 1/2$, we start with

$$A^n_\nu(\zeta,a,r) = (-1)^n\frac{\partial^n}{\partial\zeta^n}A^0_\nu(\zeta,a,r) = (-1)^n\frac{\partial^n}{\partial\zeta^n}\left[I_\nu(\zeta\rho)K_\nu(\zeta\rho')\right],$$

where $\rho = \min\{a, r\}$ and $\rho' = \max\{a, r\}$, which follows from (6) and (8). Now,

$$\frac{\partial^n}{\partial \zeta^n}\left[I_\nu(\zeta\rho)K_\nu(\zeta\rho')\right] = \sum_{i=0}^{n}\binom{n}{i}\rho^{n-i}I_\nu^{(n-i)}(\zeta\rho)\,\rho'^{i}K_\nu^{(i)}(\zeta\rho').$$

Recalling also (10), we have

$$\bar{A}_\lambda^n(a,r) = A_\nu^n(\zeta,a,r)\big|_{\zeta=1} = \begin{cases} (-1)^n\displaystyle\sum_{i=0}^{n}\binom{n}{i} r^{n-i}I_\nu^{(n-i)}(r)\,a^i K_\nu^{(i)}(a) & \text{if } r < a, \\ (-1)^n\displaystyle\sum_{i=0}^{n}\binom{n}{i} a^{n-i}I_\nu^{(n-i)}(a)\,r^i K_\nu^{(i)}(r) & \text{if } r > a. \end{cases} \tag{61}$$

Now, by (56), we have the asymptotic equalities

$$r^m I_\nu^{(m)}(r) \sim \frac{\prod_{j=1}^{m}(\nu - j + 1)}{2^\nu\Gamma(\nu+1)}\,r^\nu \quad \text{as } r \to 0, \quad m = 0, 1, \ldots,$$

and

$$r^m K_\nu^{(m)}(r) \sim (-1)^m\sqrt{\frac{\pi}{2}}\,r^{m-1/2}e^{-r} \quad \text{as } r \to \infty, \quad m = 0, 1, \ldots$$

The results in (57)–(60) follow by substituting these asymptotic equalities in (61). □

4. NUMERICAL COMPUTATION OF BCLFs

The review given in Section 2 suggests several ways of computing the BCLFs. Thus, we can compute them via the recursion relations in (13) and (14) given in Section 2.3. We can use the various explicit expressions given in Section 2.3. We can also compute the BCLFs by numerically evaluating their integral representations discussed in Section 2.4. In what follows, we evaluate the efficiency of the approaches through recursion relations and integral representations as these seem to be more convenient than explicit expressions.

4.1 Computing BCLFs by numerical quadrature

One way of computing the BCLFs is via the integral given in (31). Because the functions $I_{\lambda+1/2}(x)$ tend to infinity like $e^x/\sqrt{2\pi x}$ as $x \to \infty$, it is better

for numerical purposes to scale them with the factor e^{-x}, as a result of which, (31) becomes

$$A^n_{\lambda+1/2}(\zeta, a, r) = \frac{1}{2}\int_0^\infty u^{n/2} H_n(\zeta\sqrt{u})\left[\exp\left(-\frac{ar}{2u}\right) I_{\lambda+1/2}\left(\frac{ar}{2u}\right)\right] \exp\left[-\zeta^2 u - \frac{(a-r)^2}{4u}\right]\frac{du}{u}, \tag{62}$$

where $H_n(x)$ is the nth Hermite polynomial. Because of the homogeneity property of BCLFs given in (9), it is sufficient to treat the computation of $\bar{A}^n_\lambda(a, r)$ via

$$\bar{A}^n_\lambda(a, r) = \frac{1}{2}\int_0^\infty u^{n/2} H_n(\sqrt{u})\left[\exp\left(-\frac{ar}{2u}\right) I_{\lambda+1/2}\left(\frac{ar}{2u}\right)\right] \exp\left[-u - \frac{(a-r)^2}{4u}\right]\frac{du}{u}. \tag{63}$$

Denoting the integrand in (63) by $F(u)$ for simplicity, and taking into consideration the fact that $H_n(x)$ is even (odd) when n is even (odd), we can show that $F(u)$ is infinitely differentiable in the open interval $(0, \infty)$, while

$$F(u) \sim \begin{cases} C\, u^{\lfloor (n-1)/2\rfloor + 1/2} \exp\left[-\dfrac{(a-r)^2}{4u}\right] & \text{as } u \to 0 \\ D\, u^{n-\lambda-3/2}\exp(-u) & \text{as } u \to \infty \end{cases} \tag{64}$$

for some nonzero constants C and D. In view of this, it seems appropriate to first subdivide the interval into two, namely,

$$\int_0^\infty F(u)\, du = \int_0^R F(u)\, du + \int_R^\infty F(u)\, du, \quad \text{for some } R > 0,$$

and compute the two integrals separately by appropriate numerical quadrature methods. In particular, we can use Gauss–Laguerre quadrature to compute $\int_R^\infty F(u)\, du$, while $\int_0^R F(u)\, du$ can be computed via Gauss–Legendre quadrature. This approach to the computation of $\bar{A}^n_\lambda(a, r)$ has indeed been used in the past, e.g., in STOP by Bouferguène, Fares, and Hoggan.[7]

Since we ultimately need to sum infinite series whose terms are proportional to $\bar{A}^n_\lambda(a, r)$, and since these series may converge slowly, it is

necessary to compute $\bar{A}_\lambda^n(a,r)$, $\lambda = 0, 1, \ldots, L$, L being quite large. This will be the case even when we try to accelerate the convergence of these series by suitable extrapolation methods. (For a detailed treatment of extrapolation methods, see Sidi.[20]) For each a and r, these integrals can be computed using the *same* numerical integration procedure. This implies that $I_{\lambda+1/2}(x)$, $\lambda = 0, 1, \ldots, L$, are required at the *same* abscissae. Therefore, a procedure by which the sequence $\{I_{\lambda+1/2}(x)\}_{\lambda=0}^{L}$ can be computed for any positive x to machine accuracy in the most economical way is necessary.

However, the computation of the $\bar{A}_\lambda^n(a,r)$ with high accuracy via numerical quadrature as explained above requires many evaluations of the integrand $F(u)$, hence of the functions $I_{\lambda+1/2}(x)$. In addition, we need to monitor the convergence behavior of the numerical quadrature procedures used to make sure that machine accuracy is achieved. In view of these facts, we conclude that this way of determining the $\bar{A}_\lambda^n(a,r)$ will tend to be rather expensive.

4.2 Computing BCLFs via recursion

Computing the $\bar{A}_\lambda^n(a,r)$ by the recursion relations in (15) and (16) with the initial values in (17), on the other hand, seems to be very economical. However, when implemented in floating-point arithmetic, this approach seems to have one serious drawback, namely, a loss of accuracy takes place when computing the $\bar{A}_\lambda^{n+2}(a,r)$ from the $\bar{A}_\lambda^n(a,r)$ for increasing λ, even though the $\bar{A}_\lambda^0(a,r)$ have been determined to machine accuracy. Furthermore, this loss of accuracy becomes more pronounced as r approaches a. [Note the need to compute $\bar{A}_\lambda^n(a,r)$ for $n = 0, 1, \ldots, 6$ in order to be able to cover the whole periodic table.] The way this phenomenon comes about can be explained with the help of Theorems 3.1 and 3.2 as follows.

Let us recall that a loss of accuracy is incurred when taking the difference between two floating-point numbers that are very close to each other, and that this loss of accuracy becomes worse as the two numbers approach each other further. The loss of accuracy that is observed in computing the BCLFs via the recursion relations in (15) and (16) comes about exactly in this way. As can be concluded from the results of Theorems 3.1 and 3.2, the computation of the $\bar{A}_\lambda^n(a,r)$, $n \geq 2$, via the recursion relation in (16), whether $r \neq a$ or $r = a$, involves taking the difference of two quantities that are *asymptotically equal*[3] as $\lambda \to \infty$. Specifically, when computing

[3] Two functions $f(x)$ and $g(x)$ are said to be *asymptotically equal as* $x \to x_0$ if $\lim_{x\to x_0} f(x)/g(x) = 1$.

$\bar{A}_\lambda^{n+2}(a,r)$ via (16), we are taking the difference between the quantities $(a^2+r^2)\bar{A}_\lambda^n(a,r)$ and $\frac{2ar}{2\lambda+1}\left[\lambda\bar{A}_{\lambda-1}^n(a,r)+(\lambda+1)\bar{A}_{\lambda+1}^n(a,r)\right]$, which are asymptotically equal as $\lambda\to\infty$, as can be shown by invoking (39). In addition, when computing $\bar{A}_\lambda^1(a,a)$ via (15) with $r=a$ there, we are taking the difference between $\bar{A}_{\lambda-1}^0(a,a)$ and $\bar{A}_{\lambda+1}^0(a,a)$, which are also asymptotically equal as $\lambda\to\infty$. These explain the loss of accuracy that takes place when computing the $\bar{A}_\lambda^n(a,r)$ by recursion for large λ. This loss of accuracy is more pronounced for r very near a (and for $r=a$), because, as is suggested by Theorem 3.2, the quantities whose difference is being computed in floating-point arithmetic are asymptotically equal as $\lambda\to\infty$, more when $r=a$ than when $r\neq a$. As a result, when using a certain floating-point arithmetic, maintaining the same (machine) accuracy for all $n=0,1,\ldots,6$, becomes impossible. This problem can be overcome by carrying out the recursions with variable-precision arithmetic provided by computer algebra systems such as Maple. However, use of these systems may slow down the computations considerably, hence may not be very practical at this time. Nevertheless, this idea of using high-accuracy arithmetic is appealing, and we next discuss a practical way to overcome the timing deficiency.

When using double-precision arithmetic—which is what is normally done—this problem can be overcome by performing the computation of the $\bar{A}_\lambda^n(a,r)$ in quadruple-precision arithmetic and truncating the results to double precision only after *all* of the required $\bar{A}_\lambda^n(a,r)$ have been computed. As already mentioned, there is some loss of accuracy in going from the $\bar{A}_\lambda^n(a,r)$ to the $\bar{A}_\lambda^{n+2}(a,r)$. Specifically, $\bar{A}_\lambda^1(a,r)$ and $\bar{A}_\lambda^2(a,r)$ will have approximately the same accuracy but will be less accurate than $\bar{A}_\lambda^0(a,r)$, $\bar{A}_\lambda^3(a,r)$, and $\bar{A}_\lambda^4(a,r)$ will have approximately the same accuracy but will be less accurate than $\bar{A}_\lambda^1(a,r)$ and $\bar{A}_\lambda^2(a,r)$, $\bar{A}_\lambda^5(a,r)$ and $\bar{A}_\lambda^6(a,r)$ will have approximately the same accuracy but will be less accurate than $\bar{A}_\lambda^3(a,r)$ and $\bar{A}_\lambda^4(a,r)$, and so on. Thus, there will be only three accuracy reduction steps while computing the $\bar{A}_\lambda^n(a,r)$, $0\le n\le 6$. This means that, in the worst case, when five correct decimal digits are lost at each step, the number of correct decimal digits lost in computing the $\bar{A}_\lambda^5(a,r)$ and $\bar{A}_\lambda^6(a,r)$ will be about 15. If the $\bar{A}_\lambda^0(a,r)$ have quadruple-precision accuracy (approximately 34 correct decimal digits), all the $\bar{A}_\lambda^n(a,r)$ thus computed will end up having at least double-precision accuracy.

Even though computations in quadruple-precision arithmetic are more time consuming than in double-precision arithmetic, the cost of performing the computation of the $\bar{A}_\lambda^n(a,r)$ in quadruple-precision arithmetic in FORTRAN is negligible because the number of arithmetic operations

needed for this task is very small. In view of all this, we propose to compute the BCLFs via the recursion relations, exactly as we have just explained, with the caveat that, to avoid underflows and overflows, we will *scale* both the $\bar{A}^n_\lambda(a,r)$ and the $I_{\lambda+1/2}(x)$ and $K_{\lambda+1/2}(x)$ appropriately.

5. COMPUTATIONAL DETAILS: SCALED MODIFIED SPHERICAL BESSEL FUNCTIONS AND BCLFs

5.1 Scaled modified spherical Bessel functions

The computation of the modified spherical Bessel functions $I_{n+1/2}(x)$ and $K_{n+1/2}(x)$ has been the subject of much work, and various computer programs for it exist in the literature. See, for example, Amos.[2,3]

The procedure used for computing $I_{n+1/2}(x)$ with large n is by applying Miller's backward recursion algorithm to the three-term recursion relation satisfied by the $I_{n+1/2}(x)$, namely, to

$$I_{n+1/2}(x) - I_{n+5/2}(x) = \frac{2n+3}{x} I_{n+3/2}(x), \quad n = 0, \pm 1, \pm 2, \ldots \tag{65}$$

For the backward recursion algorithm, see, for example, Gautschi.[9]

The $K_{n+1/2}(x)$, on the other hand, can be computed by using the three-term recursion relation

$$K_{n+5/2}(x) - K_{n+1/2}(x) = \frac{2n+3}{x} K_{n+3/2}(x), \quad n = 0, \pm 1, \pm 2, \ldots, \tag{66}$$

in the forward direction.

Note that, when $x > 0$, we have $I_{n+1/2}(x) > 0$ for $n \geq -1$, while $K_{n+1/2}(x) > 0$ for $n = 0, \pm 1, \pm 2, \ldots$.

Now, $I_{n+1/2}(x)$ and $K_{n+1/2}(x)$ satisfy the well-known asymptotic equalities

$$I_\nu(x) \sim \frac{1}{\sqrt{2\pi x}} e^x \quad \text{as } x \to \infty \quad \text{and} \quad K_\nu(x) \sim \sqrt{\frac{\pi}{2x}}\, e^{-x} \quad \text{as } x \to \infty. \tag{67}$$

These show that the computation of $I_\nu(x)$ and $K_\nu(x)$ in floating-point arithmetic with very large x will ultimately result in overflows and underflows, respectively. To avoid this problem, all known codes compute $e^{-x} I_{n+1/2}(x)$ and $e^x K_{n+1/2}(x)$ and not $I_{n+1/2}(x)$ and $K_{n+1/2}(x)$.

Because we need to compute the BCLFs $\bar{A}_\lambda^n(a,r)$ for very high values of λ, we need to make sure that the large values of λ do not introduce additional problems in floating-point arithmetic. Now, as mentioned in Appendix A, the functions $I_\nu(x)$ and $K_\nu(x)$, with x fixed, satisfy the asymptotic equalities

$$I_\nu(x) \sim \frac{(x/2)^\nu}{\Gamma(\nu+1)} \quad \text{as } \nu \to \infty \quad \text{and} \quad K_\nu(x) \sim \frac{1}{2}\,\frac{\Gamma(\nu)}{(x/2)^\nu} \quad \text{as } \nu \to \infty. \tag{68}$$

It is thus clear that the computation of $I_\nu(x)$ with very large ν will ultimately result in underflows. Analogously, the computation of $K_\nu(x)$ with very large ν will ultimately result in overflows. This means that computing $e^{-x}I_{n+1/2}(x)$ and $e^{x}K_{n+1/2}(x)$, which is normally what is done as already mentioned, will not work for large n.

To avoid both of these problems as much as possible, instead of $I_{n+1/2}(x)$ and $K_{n+1/2}(x)$, which are needed in our work, we choose to compute some suitably scaled versions of them, the scaling depending on n. Specifically, we compute the functions

$$\begin{aligned} \widehat{I}_n(x) &= \frac{\Gamma(n+1/2)}{(x/2)^{n+1/2}}\, e^{-x} I_{n+1/2}(x), \\ \widehat{K}_n(x) &= \frac{(x/2)^{n+1/2}}{\Gamma(n+1/2)}\, e^{x} K_{n+1/2}(x), \quad n = 0, \pm 1, \pm 2, \ldots \end{aligned} \tag{69}$$

The complete algorithmic details of this computation are given in Appendix B.

The reader may be wondering why we chose $\Gamma(n+1/2)$, and not the simpler $\Gamma(n+1) = n!$ or $\Gamma(n+\alpha)$ for some other $\alpha \neq 1, 1/2$, to scale $I_{n+1/2}(x)$ and $K_{n+1/2}(x)$. The reasons for this are that (i) with $\Gamma(n+1)$, the $\widehat{I}_n(x)$, $n \leq -1$, are all infinite, and $\widehat{K}_n(x)$, $n \leq -1$, are all zero, and (ii) with $\alpha \neq 1, 1/2$, we need to compute $\Gamma(\alpha)$ in very high precision, which we want to avoid; on the other hand, $\Gamma(1/2) = \sqrt{\pi}$, and is readily available in every precision since $\pi = \arccos(-1)$ is.

5.2 Scaled BCLFs

Clearly, in terms of $\widehat{I}_n(x)$ and $\widehat{K}_n(x)$, $\bar{A}_\lambda^0(a,r)$ can be computed via

$$\begin{aligned} \bar{A}_\lambda^0(a,r) &= (\rho/\rho')^{\lambda+1/2} e^{\rho-\rho'} C_\lambda^0(a,r); \quad C_\lambda^0(a,r) = \widehat{I}_\lambda(\rho)\, \widehat{K}_\lambda(\rho'), \\ &\rho = \min\{a,r\}, \quad \rho' = \max\{a,r\}. \end{aligned} \tag{70}$$

With the $C_\lambda^0(a,r)$ already computed as in (70), we compute $C_\lambda^n(a,r)$, $n=1,2,\ldots$, via the recursions

$$C_\lambda^1(a,r)=\frac{ar}{2\lambda+1}\left[(\rho/\rho')^{-1}C_{\lambda-1}^0(a,r)-(\rho/\rho')C_{\lambda+1}^0(a,r)\right], \quad (71)$$

$$C_\lambda^{n+2}(a,r)=(a^2+r^2)C_\lambda^n(a,r)-\frac{2ar}{2\lambda+1}\Big[\lambda(\rho/\rho')^{-1}C_{\lambda-1}^n(a,r) + (\lambda+1)(\rho/\rho')C_{\lambda+1}^n(a,r)\Big], \quad n\geq 0. \quad (72)$$

Then, for all $n\geq 0$, we have

$$\bar{A}_\lambda^n(a,r)=(\rho/\rho')^{\lambda+1/2}e^{\rho-\rho'}C_\lambda^n(a,r); \quad \rho=\min\{a,r\}, \quad \rho'=\max\{a,r\}. \quad (73)$$

We shall call the $C_\lambda^n(a,r)$ *scaled BCLFs*.

When $r\gg a$, the factors $(\rho/\rho')^{\lambda+1/2}$ and $e^{\rho-\rho'}$ in (73) are very small and thus can cause underflows. To avoid this problem, we should keep the three factors $(\rho/\rho')^{\lambda+1/2}$, $e^{\rho-\rho'}$, and $C_\lambda^n(a,r)$ as separate entities. It may be even a better idea not to compute $(\rho/\rho')^{\lambda+1/2}$ and $e^{\rho-\rho'}$ right away, but to incorporate them in whatever computation is done with $\bar{A}_\lambda^n(a,r)$, in an appropriate manner that will avoid underflows.

Before closing, we report the results of some computations we have performed with the recursion relation above. These computations confirm the conclusions we arrived at above concerning the achievable accuracy of the BCLFs via the recursion relation. Let us define ε to be the relative error incurred when computing $\bar{A}_\lambda^n(a,r)$ in quadruple-precision arithmetic. Thus,

$$\varepsilon=\max\left\{\left|\frac{\nu_{\text{app}}-\nu_{\text{ex}}}{\nu_{\text{ex}}}\right|, 10^{-32}\right\}, \quad (74)$$

where ν_{app} is the (approximate) value computed in quadruple-precision and ν_{ex} is the exact value computed with much more precision within a computer algebra system. Figures 3.1 and 3.2 show the graphs of $-\log_{10}\varepsilon$ versus λ, for $a=2.5$ and $r=1.0, 2.5$, when $0\leq\lambda\leq 150$. Note the lower accuracy achieved for $r=a=2.5$ in Figure 3.2.

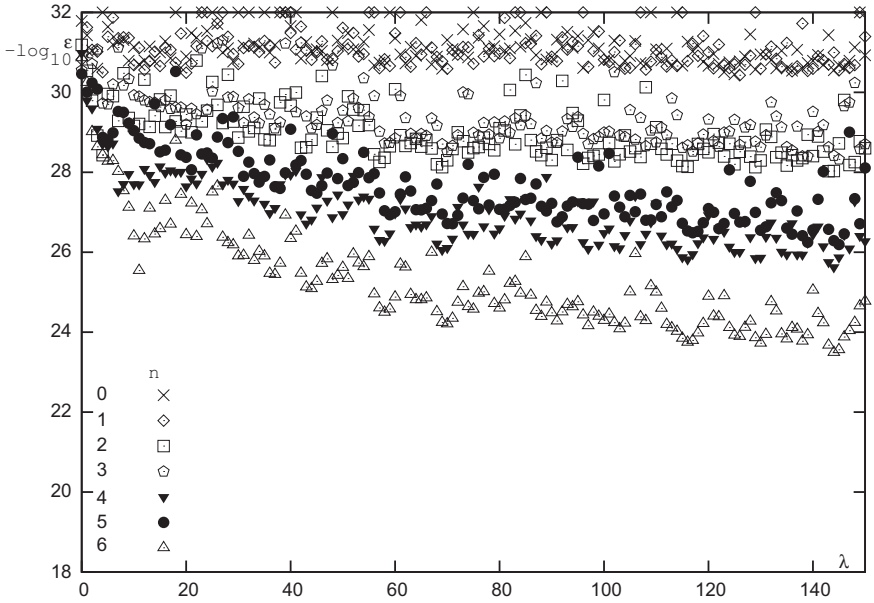

Figure 3.1 Relative error in quadruple-precision computation of $\bar{A}^n_\lambda(a,r)$ for $a = 2.5, r = 1.0$ as a function of λ.

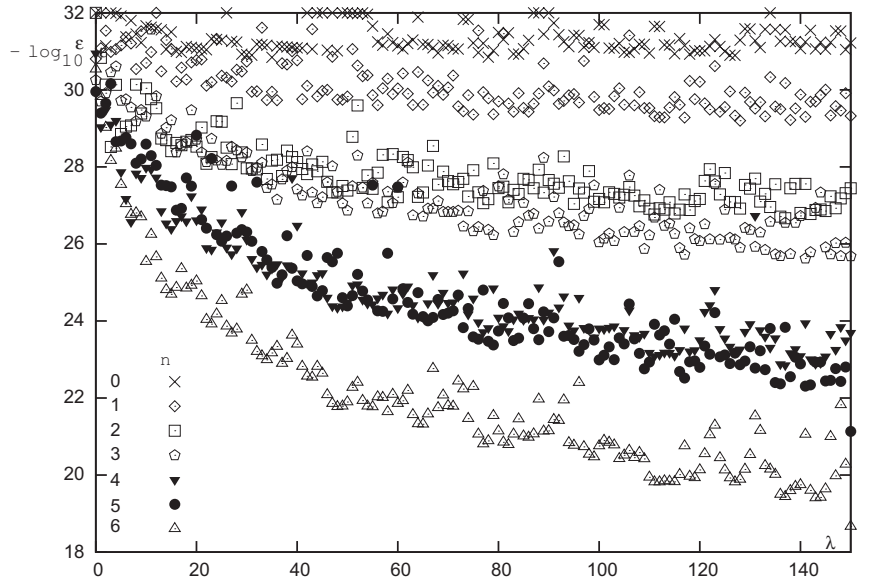

Figure 3.2 Relative error in quadruple-precision computation of $\bar{A}^n_\lambda(a,r)$ for $a = 2.5, r = 2.5$ as a function of λ.

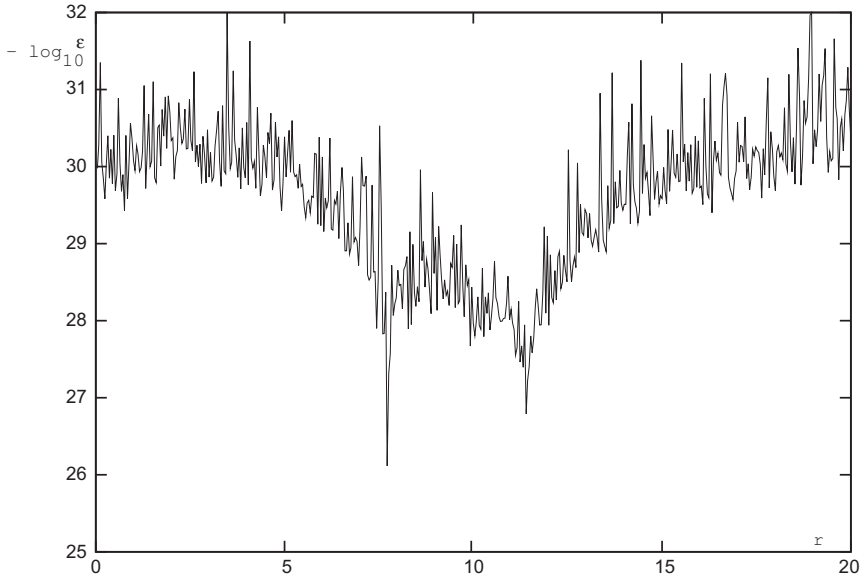

Figure 3.3 Relative error in quadruple-precision computation of $\bar{A}_\lambda^n(a,r)$ for $n = 3, \lambda = 10, a = 10.0$, as a function of r.

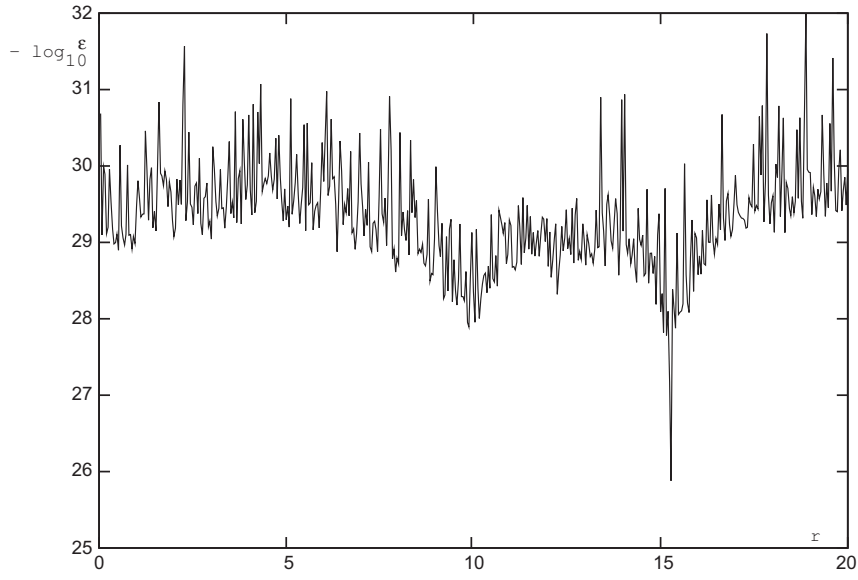

Figure 3.4 Relative error in quadruple-precision computation of $\bar{A}_\lambda^n(a,r)$ for $n = 3, \lambda = 25, a = 10.0$, as a function of r.

Figures 3.3 and 3.4 show the variation of the relative error when computing $\bar{A}_\lambda^n(a,r)$ with $n=3$ and $a=10.0$, as a function of r, $0<r\le 20.0$, for $\lambda=10$ and $\lambda=25$. Each graph is obtained with 500 evenly distributed values of r in the interval $[0,20.0]$. Note the lower precision achieved for $r\approx a=10.0$ in both figures. Also observe the downward peaks, which correspond to zeros of $\bar{A}_\lambda^n(a,r)$ for $n=3$ and $a=10.0$. These zeros are at $r=7.7194995476864$ and $r=11.3859436108731$ for $\lambda=10$, and at $r=15.2818830196746$ for $\lambda=25$.

APPENDIX A. ASYMPTOTIC EXPANSIONS FOR $I_\nu(z)$, $K_\nu(z)$, AND $I_\nu(z)K_\nu(z)$ AS $\nu\to\infty$

The asymptotic analysis of BCLFs is made possible by the asymptotics of the modified spherical Bessel functions $I_{n+1/2}(z)$ and $K_{n+1/2}(z)$ as $n\to\infty$. These follow immediately from the asymptotic expansions of the modified Bessel functions $I_\nu(z)$ and $K_\nu(z)$ as $\nu\to\infty$, derived in the recent paper by Sidi and Hoggan[22] for complex z and complex ν. We provide these in Theorems A.1 and A.2 that follow. (See also Sidi Ref. 21, Section 4, Example 4.1, which was used in[22] for completing the proof of Theorem A.1.)

Theorem A.1 *Define the set $T_+(\epsilon)$ via*

$$T_+(\epsilon)=\left\{\nu:\ |\nu+n|\ge\epsilon;\quad n=0,1,2,\ldots,\quad \epsilon\in\left(0,\tfrac{1}{2}\right)\right\}. \tag{A.1}$$

Then, for fixed $z\neq 0$, and $|\arg z|<\pi$, the principal values of the modified Bessel functions $I_\nu(z)$ and $K_\nu(z)$ have the asymptotic expansions

$$I_\nu(z)\sim\frac{(\frac{1}{2}z)^\nu}{\Gamma(\nu+1)}\sum_{m=0}^{\infty}\frac{b_m(z)}{\nu^m}\quad\text{as }\nu\to\infty,\quad \nu\in T_+(\epsilon), \tag{A.2}$$

and

$$K_\nu(z)\sim\frac{1}{2}\frac{\Gamma(\nu)}{(\frac{1}{2}z)^\nu}\sum_{m=0}^{\infty}(-1)^m\frac{b_m(z)}{\nu^m}\quad\text{as }\nu\to\infty,\quad |\arg\nu|\le\tfrac{1}{2}\pi-\delta, \tag{A.3}$$

where $\delta > 0$ is arbitrarily small, and for each $m = 0, 1, \ldots, b_m(z)$ is a polynomial of degree m in z^2, given as in

$$b_0(z) = 1; \quad b_m(z) = \sum_{k=1}^{m} (-1)^{m-k} \frac{S(m,k)}{k!} \left(\tfrac{1}{4}z^2\right)^k, \quad m = 1, 2, \ldots. \tag{A.4}$$

Here S(m,k) are Stirling numbers of the second kind. [Note that the $b_m(z)$ in (A.2) and (A.3) are identical and, for each m, the coefficients of $b_m(z)$ have alternating signs.]

Note. The *Stirling numbers of the second kind* $S(n,k)$ are defined via the recursion relation

$$S(n,k) = S(n-1,k-1) + kS(n-1,k), \quad n = 1, 2, \ldots, \quad k = 0, 1, \ldots, \tag{A.5}$$

with

$$S(n,0) = \begin{cases} 1 \text{ if } n = 0 \\ 0 \text{ if } n > 0 \end{cases}; \quad S(n,1) = 1, \quad n \geq 1; \tag{A.6}$$
$$S(n,n) = 1, \quad n = 0, 1, \ldots; \quad S(n,k) = 0 \quad \text{if } n < k \text{ or } n < 0.$$

Note also that $S_{n,k} > 0$ for all $k \geq n \geq 1$. They are generated as in

$$\frac{1}{(\zeta+1)_k} = \sum_{n=k}^{\infty} (-1)^{n-k} S(n,k) \zeta^{-n}, \quad |\zeta| > k. \tag{A.7}$$

See, for example, Graham, Knuth, and Patashnik [Ref. 11, Sections 6.1 and 7.4].

Theorem A.2 *For fixed $z \neq 0$, the product $I_\nu(z)K_\nu(z)$ has the asymptotic expansion*

$$I_\nu(z)K_\nu(z) \sim \frac{1}{2\nu} \sum_{s=0}^{\infty} \frac{p_s(z)}{\nu^{2s}} \quad \text{as } \nu \to \infty, \quad |\arg \nu| \leq \tfrac{1}{2}\pi - \delta, \tag{A.8}$$

where $p_s(z)$ is a polynomial of degree s in z^2, given by

$$p_0(z) = 1; \quad p_s(z) = \sum_{k=1}^{s} \gamma_{s,k} w^k, \quad s = 1, 2, \ldots,; \quad w = \tfrac{1}{4}z^2, \tag{A.9}$$

where

$$\gamma_{s,k} = (-1)^k \binom{2s}{2k} \binom{2k}{k} B_{2s-2k}^{(-2k)}(-k), \quad k = 1, \ldots, s. \tag{A.10}$$

Moreover, $(-1)^k \gamma_{s,k} > 0, k = 1, \ldots, s$. *Here,* $B_k^{(a)}(u)$ *are generalized Bernoulli polynomials.*

Note. The *generalized Bernoulli polynomials* $B_k^{(a)}(u)$ are defined via

$$\left(\frac{t}{e^t - 1}\right)^a e^{ut} = \sum_{k=0}^{\infty} B_k^{(a)}(u) \frac{t^k}{k!}, \quad |t| < 2\pi. \tag{A.11}$$

Of course, $B_k^{(a)}(u)$ is of degree k in u, and $B_0^{(a)}(u) = 1$. These polynomials satisfy

$$B_k^{(a)}(a - u) = (-1)^k B_k^{(a)}(u), \quad k = 0, 1, \ldots, \tag{A.12}$$

from which we also have $B_{2k+1}^{(a)}(\frac{1}{2}a) = 0, k = 0, 1, \ldots$. The constants $B_k^{(a)}(0)$ are called *generalized Bernoulli numbers* and they are denoted simply by $B_k^{(a)}$. Note that (A.11) is valid also when $a = u = 0$, in which case $B_0^{(0)}(0) = 1$ and $B_k^{(0)}(0) = 0, k = 1, 2, \ldots$. Note that $B_{2k}^{(a)}(\frac{1}{2}a) > 0, k = 0, 1, \ldots$, when a is a negative integer. To see this, we note that with $a = -r$ and $u = \frac{1}{2}a$, where r is a positive integer, we have

$$\left(\frac{t}{e^t - 1}\right)^a e^{ut} = \left(\frac{\sinh(\frac{1}{2}t)}{\frac{1}{2}t}\right)^r.$$

Since $\xi^{-1} \sinh \xi$ has a Maclaurin expansion in ξ with only even powers and positive coefficients, so does its rth power. For more information on generalized Bernoulli polynomials, see [Ref. 18, pp. 18–22], for example.

APPENDIX B. COMPUTATION OF SCALED $I_{n+1/2}(x)$ AND $K_{n+1/2}(x)$

B.1 Computation of the $\widehat{I}_n(x)$

Letting $I_{n+1/2}(x) = e^x \widehat{I}_n(x)(x/2)^{n+1/2}/\Gamma(n + 1/2)$ in (65), and making use of the fact that $\Gamma(z + 1) = z\Gamma(z)$, we obtain the recursion relation

$$\widehat{I}_n(x) = \frac{1}{n+1/2}\left[(n+3/2)\,\widehat{I}_{n+1}(x) + \frac{(x/2)^2}{n+3/2}\,\widehat{I}_{n+2}(x)\right], \quad n = 0, \pm 1, \pm 2, \ldots \tag{B.1}$$

We also have the power series representation

$$I_\nu(x) = \sum_{k=0}^{\infty} \frac{(x/2)^{\nu+2k}}{k!\,\Gamma(\nu+k+1)} \tag{B.2}$$

that is valid for all $\nu \neq -1, -2, \ldots$, and that converges very quickly for small x. From this, and by $\Gamma(\nu+k) = (\nu)_k \Gamma(\nu)$, where $(u)_k = \prod_{i=1}^{k}(u+i-1)$ is the Pochhammer symbol, we obtain the following series representation for $\widehat{I}_n(x)$:

$$\widehat{I}_n(x) = \frac{e^{-x}}{n+1/2} \sum_{k=0}^{\infty} \frac{(x/2)^{2k}}{k!\,(n+3/2)_k}, \quad n = 0, \pm 1, \pm 2, \ldots. \tag{B.3}$$

Note that the terms of the infinite series in (B.2) with $\nu = n+1/2$ and in (B.3) are all positive for $n \geq -1$ when $x > 0$. Therefore, when $x > 0$, $I_{n+1/2}(x) > 0$ for $n \geq -1$, and $\widehat{I}_{-1}(x) < 0$ and $\widehat{I}_n(x) > 0$ for $n \geq 0$.

We now describe the method of computing the functions $\widehat{I}_n(x)$, $n = 0, \pm 1, \pm 2, \ldots$, that we propose. We need to compute these for $-l \leq n \leq L$, where l is a small positive integer (for example $l = 5$), while L is a large positive integer. Here are the steps of this method:

1. For small positive x, say $x < 1$, $\widehat{I}_n(x)$ can be computed by summing the infinite series in (B.3). Because it converges very fast, only very few terms of this series suffice for obtaining quadruple-precision accuracy for $\widehat{I}_n(x)$ for all x. Actually, the number of terms needed for this purpose decreases with increasing n. In addition, its terms $c_{n,k}(x) = \frac{(x/2)^{2k}}{k!\,(n+3/2)_k}$ can be obtained inexpensively by the simple recursion

$$c_{n,k}(x) = c_{n,k-1}(x)\frac{(x/2)^2}{k(n+k+1/2)}, \quad k = 1, 2, \ldots; \quad c_{n,0}(x) = 1. \tag{B.4}$$

2. For other (larger) values of x, we proceed as follows. We pick an integer M that is larger than L, and set $a_M(x) = 0$ and $a_{M-1}(x) = 1$. Then compute $a_n(x)$, $-l \leq n \leq M-2$, via the backward recursion

$$a_n(x) = \frac{1}{n+1/2}\left[(n+3/2)\,a_{n+1}(x) + \frac{(x/2)^2}{n+3/2}\,a_{n+2}(x)\right],$$
$$n = M-2, M-3, \ldots, 1, 0, -1, \ldots, -l. \tag{B.5}$$

Following this, we compute

$$\widehat{a}_n^{(M)}(x) = \frac{a_n(x)}{a_0(x)}\,\widehat{I}_0(x), \quad n = -l, -l+1, \ldots, \ldots, L, \tag{B.6}$$

and take $\widehat{a}_n^{(M)}(x)$ as our approximation to $\widehat{I}_n(x)$ for $-l \le n \le L$. This is allowed since (i) $a_0(x) > 0$ for $x > 0$, which follows directly from (B.5), and (ii) $\widehat{I}_0(x) > 0$ for $x > 0$ by the fact that

$$\widehat{I}_0(x) = \frac{\Gamma(1/2)}{(x/2)^{1/2}}\,e^{-x} I_{1/2}(x) = 2e^{-x}\frac{\sinh x}{x}.$$

Of course, $\widehat{a}_0^{(M)}(x) = \widehat{I}_0(x)$ exactly. In order to avoid problems in floating-point arithmetic (especially, overflows for large x, and loss of significance for small x), we must compute $\widehat{I}_0(x)$ as in

$$\widehat{I}_0(x) = \begin{cases} 2\,e^{-x}\,\dfrac{\sinh x}{x} & \text{for small } x \\ \dfrac{1-e^{-2x}}{x} & \text{for large } x. \end{cases} \tag{B.7}$$

Note also that, as is clear from (B.5), in backward recursion with $n \ge -1$, we are adding floating-point numbers that are positive; therefore, no loss of significance takes place in the process of computing the $a_n(x)$. Clearly, $a_{-1}^{(M)}(x) < 0$, and $a_n^{(M)}(x) > 0$ for $0 \le n < M$, as can be seen from (B.5) and (B.6).

B.2 Computation of the $\widehat{K}_n(x)$

Letting $K_{n+1/2}(x) = e^{-x}\widehat{K}_n(x)\Gamma(n+1/2)/(x/2)^{n+1/2}$ in (66), and again making use of the fact that $\Gamma(z+1) = z\Gamma(z)$, we obtain the recursion relation

$$\widehat{K}_{n+2}(x) = \frac{(x/2)^2}{(n+1/2)(n+3/2)}\,\widehat{K}_n(x) + \widehat{K}_{n+1}(x), \quad n = 0, \pm 1, \pm 2, \ldots \tag{B.8}$$

By (6), we need to compute $\widehat{K}_{n+1/2}(x)$ for $x = \zeta \max\{a, r\} \geq \zeta a$. Because ζ and a are fixed and not small, it is clear that we do not need to compute $\widehat{K}_{n+1/2}(x)$ for small x. For all other values of x, $\widehat{K}_n(x), 2 \leq n \leq L$, can be computed with machine accuracy from (B.8) by forward recursion, with

$$\begin{aligned} \widehat{K}_0(x) &= \frac{(x/2)^{1/2}}{\Gamma(1/2)}\, e^x K_{1/2}(x) = \frac{1}{2} \quad \text{and} \\ \widehat{K}_1(x) &= \frac{(x/2)^{3/2}}{\Gamma(3/2)}\, e^x K_{3/2}(x) = \frac{1}{2}\,(1+x) \end{aligned} \tag{B.9}$$

as initial values. To compute $\widehat{K}_n(x), -l \leq n \leq -1$, we use (B.8) in the backward direction, with $\widehat{K}_0(x)$ and $\widehat{K}_1(x)$ as initial values again.

Note that, making use of the fact that

$$K_{-p-1/2}(x) = K_{p+1/2}(x), \quad p = 0, 1, \ldots, \tag{B.10}$$

we can also compute $\widehat{K}_n(x), -l \leq n \leq -1$, via

$$\begin{aligned} \widehat{K}_{-p}(x) &= \frac{(x/2)^{-p+1/2}}{\Gamma(-p+1/2)}\, e^x K_{-p+1/2}(x) \\ &= \frac{(x/2)^{-p+1/2}}{\Gamma(-p+1/2)}\, e^x K_{p-1/2}(x) \\ &= \frac{\Gamma(p-1/2)}{\Gamma(-p+1/2)}\, (x/2)^{-2p+1} \widehat{K}_{p-1}(x), \quad p = 1, 2, \ldots \end{aligned} \tag{B.11}$$

APPENDIX C. ERROR ANALYSIS

We now turn to the analysis of the errors incurred in approximating $\widehat{I}_n(x)$ and $\widehat{K}_n(x)$ as explained in the preceding section. For $\widehat{I}_n(x)$, which are computed by backward recursion, we would like to bound the error $\widehat{I}_n(x) - \widehat{a}_n^{(M)}(x)$ in $\widehat{a}_n^{(M)}(x)$ for large M. For $\widehat{K}_n(x)$, we would like to bound the error $\widehat{K}_n(x) - c_n(x)$ in $c_n(x)$, where $c_n(x)$ replaces $\widehat{K}_n(x)$ in (B.8), with $c_i(x) = (1+\epsilon_i)\widehat{K}_i(x), i = 0, 1$, as initial values with relative errors ϵ_i. In this analysis, we assume that all computations are performed with infinite precision. To be able to carry out this analysis in a refined way, we need the asymptotic behaviors of the functions $I_\nu(x)$ and $K_\nu(x)$ as $\nu \to +\infty$, when x is fixed, which are provided in Appendix A.

C.1 Error bounds for $\widehat{I}_n(x)$ approximations

We start by noting that $f_n(x) = I_{n+1/2}(x)$ and $f_n(x) = (-1)^{n+1}K_{n+1/2}(x)$ are two linearly independent solutions of the recursion relation (see Abramowitz and Stegun [Ref. 1, p. 444])

$$f_n(x) - f_{n+2}(x) = \frac{2n+3}{x} f_{n+1}(x), \quad n = 0, \pm 1, \pm 2, \ldots \tag{C.1}$$

Hence

$$\widehat{I}_n(x) = \frac{\Gamma(n+1/2)}{(x/2)^{n+1/2}}\, e^{-x} I_{n+1/2}(x)$$
$$\widehat{H}_n(x) = (-1)^{n+1}\frac{\Gamma(n+1/2)}{(x/2)^{n+1/2}}\, e^{-x} K_{n+1/2}(x)$$

are two linearly independent solutions of the recursion relation in (B.5). Therefore, every solution of (B.5) has the form

$$a_n(x) = A\widehat{I}_n(x) + B\widehat{H}_n(x), \quad n = 0, \pm 1, \pm 2, \ldots, \tag{C.2}$$

A and B being some functions of x that are independent of n. Invoking the initial conditions $a_M(x) = 0$ and $a_{M-1}(x) = 1$ with some suitably chosen large positive integer M, we obtain the following equations for A and B:

$$A\widehat{I}_M(x) + B\widehat{H}_M(x) = 0,$$
$$A\widehat{I}_{M-1}(x) + B\widehat{H}_{M-1}(x) = 1.$$

Solving these equations by Cramer's rule and noting that

$$I_{n+1/2}(x)K_{n-1/2}(x) + I_{n-1/2}(x)K_{n+1/2}(x) = \frac{1}{x} \quad \text{for all } n, \tag{C.3}$$

we obtain

$$A = -\frac{\widehat{H}_M}{\Delta}, \quad B = \frac{\widehat{I}_M}{\Delta}; \quad \Delta = (-1)^M \frac{\Gamma(M+1/2)\Gamma(M-1/2)}{(x/2)^{2M}}\, \frac{e^{-2x}}{x}.$$

Substituting these in (C.2), and invoking (B.6), we obtain

$$a_n^{(M)}(x) = \widehat{I}_n(x)\frac{1-\dfrac{\widehat{I}_M(x)}{\widehat{H}_M(x)}\dfrac{\widehat{H}_n(x)}{\widehat{I}_n(x)}}{1-\dfrac{\widehat{I}_M(x)}{\widehat{H}_M(x)}\dfrac{\widehat{H}_0(x)}{\widehat{I}_0(x)}}, \quad n = 0, \pm 1, \pm 2, \ldots, \tag{C.4}$$

from which we have the relative error

$$\frac{a_n^{(M)}(x) - \widehat{I}_n(x)}{\widehat{I}_n(x)} = \frac{\dfrac{\widehat{H}_0(x)}{\widehat{I}_0(x)} - \dfrac{\widehat{H}_n(x)}{\widehat{I}_n(x)}}{1-\dfrac{\widehat{I}_M(x)}{\widehat{H}_M(x)}\dfrac{\widehat{H}_0(x)}{\widehat{I}_0(x)}}\frac{\widehat{I}_M(x)}{\widehat{H}_M(x)}, \quad n = 0, \pm 1, \pm 2, \ldots, \tag{C.5}$$

Therefore, for n fixed, there holds

$$\frac{a_n^{(M)}(x) - \widehat{I}_n(x)}{\widehat{I}_n(x)} = O\left(\frac{\widehat{I}_M(x)}{\widehat{H}_M(x)}\right) = O\left(\frac{I_{M+1/2}(x)}{K_{M+1/2}(x)}\right) \quad \text{as } M \to \infty, \quad n = 0, \pm 1, \pm 2, \ldots \tag{C.6}$$

By (68) and by the fact that (see [Ref. 1, p. 257, Eq. 6.1.47])

$$\frac{\Gamma(z+a)}{\Gamma(z+b)} \sim z^{a-b} \quad \text{as } z \to \infty,$$

we have $I_{n+1/2}(x)/K_{n+1/2}(x) = O((x/2)^{2n}/(n!)^2)$ as $n \to \infty$. Consequently, (C.6) becomes

$$\frac{a_n^{(M)}(x) - \widehat{I}_n(x)}{\widehat{I}_n(x)} = O\left(\frac{(x/2)^{2M}}{(M!)^2}\right) \quad \text{as } M \to \infty, \quad n = 0, \pm 1, \pm 2, \ldots \tag{C.7}$$

It is clear from (C.7) that, with x fixed, the relative error in $a_n^{(M)}(x)$ is tending to zero very quickly as $M \to \infty$. Hence backward recursion indeed provides a very effective means of computing $\widehat{I}_n(x)$, $-l \le n \le L$, for some specified large L. Note that the number of arithmetic operations for achieving this task is at most of the order of $2M$ additions, $2M$ multiplications, and M divisions. Our computations show that, except for a few of the $\widehat{a}_n^{(M)}(x)$ with n very close to M, the rest of the $\widehat{a}_n^{(M)}(x)$ can be obtained to machine

precision. For example, in quadruple-precision arithmetic, by choosing $M = 150$, we are able to approximate $\widehat{I}_n(x)$ via $\widehat{a}_n^{(M)}(x)$, $-5 \le n \le 145$, to machine accuracy for all $x \ge 0.1$.

C.2 Error bounds for $\widehat{K}_n(x)$ approximations

In analogy to what we did for $\widehat{I}_n(x)$ in the preceding subsection, we start by noting that $g_n(x) = (-1)^n I_{n+1/2}(x)$ and $g_n(x) = K_{n+1/2}(x)$ are two linearly independent solutions of the recursion relation

$$g_{n+2}(x) - g_n(x) = \frac{2n+3}{x} g_{n+1}(x), \quad n = 0, \pm 1, \pm 2, \ldots \tag{C.8}$$

Hence

$$\widehat{J}_n(x) = (-1)^n \frac{(x/2)^{n+1/2}}{\Gamma(n+1/2)} e^x I_{n+1/2}(x)$$
$$\widehat{K}_n(x) = \frac{(x/2)^{n+1/2}}{\Gamma(n+1/2)} e^x K_{n+1/2}(x)$$

are two linearly independent solutions of the recursion relation

$$c_{n+2}(x) = \frac{(x/2)^2}{(n+1/2)(n+3/2)} c_n(x) + c_{n+1}(x), \quad n = 0, \pm 1, \pm 2, \ldots, \tag{C.9}$$

because (C.9) is obtained from (C.8) by letting $g_n(x) = [\Gamma(n+1/2)/(x/2)^{n+1/2}]e^{-x} c_n(x)$. Therefore,

$$c_n(x) = A\widehat{J}_n(x) + B\widehat{K}_n(x), \quad n = 0, \pm 1, \pm 2, \ldots, \tag{C.10}$$

A and B being some functions of x that are independent of n. Invoking the initial conditions $c_0(x) = (1+\epsilon_0)\widehat{K}_0(x)$ and $c_1(x) = (1+\epsilon_1)\widehat{K}_1(x)$, where ϵ_0 and ϵ_1 are the relative errors in $c_0(x)$ and $c_1(x)$ satisfying $|\epsilon_0| \le \widehat{\epsilon}$ and $|\epsilon_1| \le \widehat{\epsilon}$, we obtain the following equations for A and B:

$$A\widehat{J}_0(x) + B\widehat{K}_0(x) = (1+\epsilon_0)\widehat{K}_0(x),$$
$$A\widehat{J}_1(x) + B\widehat{K}_1(x) = (1+\epsilon_1)\widehat{K}_1(x).$$

Solving these equations by Cramer's rule and noting (C.3), we obtain

$$A = \frac{(\epsilon_0 - \epsilon_1)\widehat{K}_0(x)\widehat{K}_1(x)}{\Delta}, \quad B = 1 + \frac{\epsilon_1 \widehat{J}_0(x)\widehat{K}_1(x) - \epsilon_0 \widehat{J}_1(x)\widehat{K}_0(x)}{\Delta};$$
$$\Delta = \frac{(x/2)^2}{\Gamma(1/2)\Gamma(3/2)} \frac{e^{2x}}{x} = \frac{x}{2\pi} e^{2x}.$$

Now, the expression for the relative error in $c_n(x)$ is

$$\frac{c_n(x) - \widehat{K}_n(x)}{\widehat{K}_n(x)} = A\frac{\widehat{J}_n(x)}{\widehat{K}_n(x)} + (B-1) \quad n = 0, \pm 1, \pm 2, \ldots \tag{C.11}$$

By the fact that $I_{n+1/2}(x)$ and $K_{n+1/2}(x), n = 0, 1, \ldots$, are all positive, we have that

$$|A| \le 2xK_{1/2}(x)K_{3/2}(x)\widehat{\epsilon}, \quad |B-1| \le \widehat{\epsilon}\left[\widehat{J}_0(x)\widehat{K}_1(x) + \widehat{J}_1(x)|\widehat{K}_0(x)\right]/|\Delta| = \widehat{\epsilon},$$

from which we have

$$\left|\frac{c_n(x) - \widehat{K}_n(x)}{\widehat{K}_n(x)}\right| \le \left[2xK_{1/2}(x)K_{3/2}(x)\frac{I_{n+1/2}(x)}{K_{n+1/2}(x)} + 1\right]\widehat{\epsilon}, \quad n = 0, 1, 2, \ldots \tag{C.12}$$

Because $I_{n+1/2}(x)/K_{n+1/2}(x) = O((x/2)^{2n}/(n!)^2)$ as $n \to \infty$, it follows from (C.12) that forward recursion is very stable and accurate for $\widehat{K}_n(x)$ with large n. If $c_0(x)$ and $c_1(x)$ have machine precision, then $\widehat{\epsilon}$ is simply the roundoff unit of the floating-point arithmetic being used, hence $c_n(x)$ approximate $\widehat{K}_n(x)$ for all large n with machine precision as well.

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