Computing Solutions of the Modified Bessel Differential Equation for Imaginary Orders and Positive Arguments

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We describe a variety of methods to compute the functions $K_{ia}(x)$, $L_{ia}(x)$ and their derivatives for real a and positive x. These functions are numerically satisfactory independent solutions of the differential equation $x^2w'' + xw' + (a^2 - x^2)w = 0$. In the accompanying paper [Gil et al. 2004], we describe the implementation of these methods in Fortran 77 codes.

Categories and Subject Descriptors: G.4 [**Mathematical Software**]

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1. INTRODUCTION

In previous publications [Gil et al. 2002a, 2003], we described methods to compute the modified Bessel function $K_{ia}(x)$ for positive x. We complete this analysis here by describing analogous methods for the computation of the function $L_{ia}(x)$. With this, methods for the reliable computation of a pair of linearly independent numerically satisfactory solutions become available which find their

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implementation in the accompanying paper [Gil et al. 2004]. Methods to compute their derivatives are also provided.

The functions $K_{ia}(x)$ and $L_{ia}(x)$ are solutions of the modified Bessel equation for imaginary orders

$$x^2w'' + xw' + (a^2 - x^2)w = 0. \tag{1}$$

The function $K_{ia}(x)$ finds application in a number of problems of physics and applied mathematics [Gil et al. 2002a]. The function $L_{ia}(x)$ is a real valued numerically satisfactory companion to $K_{ia}(x)$ in the sense described in Olver [1997], pp. 154–155.

In terms of the modified Bessel function of the first kind $I_\nu(x)$, the solutions are defined as:

$$K_{ia}(x) = \frac{\pi}{2i\sinh(\pi a)}[I_{-ia}(x) - I_{ia}(x)], \quad L_{ia}(x) = \frac{1}{2}[I_{-ia}(x) + I_{ia}(x)], \tag{2}$$

with Wronskian $W[K_{ia}(x), L_{ia}(x)] = 1/x$.

Both $K_{ia}(x)$ and $L_{ia}(x)$ are real solutions for real $x > 0$ and $a \in \mathbb{R}$. Because they are even functions of a, in the sequel we will consider $a \geq 0$, although this restriction is not present in the code.

In Section 2, we describe the different methods of computation considered, namely: series expansions, asymptotic expansions for large x, Airy-type uniform asymptotic expansions, non-oscillating integral representations (including a discussion on the quadrature rule) and a continued fraction method. We avoid duplicating information already given in previous papers; in particular, the references Gil et al. [2002a, 2003] provide information required for building the algorithms of the accompanying paper [Gil et al. 2004]. A few misprints in [Gil et al. 2002a] are corrected.

In Section 3, we include a discussion on the dominant asymptotic behaviour of the functions. These exponential dominant factors can be taken out, leading to scaled functions that can be computed in a much wider range. The algorithm described in the accompanying paper [Gil et al. 2004] offers the possibility of computing scaled and unscaled functions.

2. METHODS OF COMPUTATION

In Gil et al. [2002a, 2003] methods are described to compute the $K_{ia}(x)$ for different regions in the (x, a) plane. In particular, we considered series expansions [Temme 1975], asymptotic expansions for large x [Abramowitz and Stegun 1964, Eq. 9.7.2], uniform asymptotic expansions for $a \simeq x$ [Balogh 1967; Dunster 1990; Olver 1997, pg. 425]. Also, non-oscillating integral representations [Temme 1994; Gil et al. 2002a] are available. Similar techniques are available for the computation of $L_{ia}(x)$ and the derivatives $K'_{ia}(x)$, $L'_{ia}(x)$. In addition, a continued fraction method can be applied for the computation of $K_{ia}(x)$ and $K'_{ia}(x)$. Those techniques generally give at least two alternative methods for computing the functions in the (x, a) plane for moderate values of x and a; therefore, we can always compare different methods of computation for testing their accuracy. The selection of one or another method of computation in a given region will depend on the range of applicability of each method and its efficiency.

We now describe the different methods of computation that are used in the programs.

2.1 Series Expansions

Series expansions can be built that properly describe the solutions near the singular point ($x = 0$) of the defining differential equation (1). The idea, as described in Temme [1975] and Gil et al. [2002a], is to substitute the Maclaurin series for $I_\nu(x)$ [Abramowitz and Stegun 1964, Eq. 9.6.10] in Eqs. (2). The following expansions are obtained

$$\begin{aligned} K_{ia}(x) &= \frac{1}{n(a)}\sum_{k=0}^{\infty} f_k c_k,\ K'_{ia}(x) = \frac{1}{n(a)}\frac{2}{x}\sum_{k=0}^{\infty}\left[k f_k - \frac{r_k}{2}\right]c_k \\ L_{ia}(x) &= n(a)\sum_{k=0}^{\infty} r_k c_k,\ L'_{ia}(x) = n(a)\frac{2}{x}\sum_{k=0}^{\infty}\left[k r_k + a^2\frac{f_k}{2}\right]c_k, \end{aligned} \tag{3}$$

where

$$n(a) = e^{\pi a/2}\sqrt{\frac{1-e^{-2\pi a}}{2\pi a}}, \quad c_k = (x/2)^{2k}/k! \tag{4}$$

and [Dunster 1990]

$$\begin{aligned} f_k &= \frac{\sin(\phi_{a,k} - a\ln(x/2))}{(a^2(1+a^2)\cdots(k^2+a^2))^{1/2}}, \\ f_k/r_k &= \frac{1}{a}\tan(\phi_{a,k} - a\ln(x/2)),\ \text{with } \phi_{a,k} = \arg(\Gamma(1+k+ia)). \end{aligned} \tag{5}$$

The coefficients f_k and r_k differ from those in Gil et al. [2002a] by a constant factor (for fixed a). The new normalization shows explicitly (Eqs. (3)) the dominant exponential behaviour $n(a)$ and $1/n(a)$ as $a \to \infty$ ($\sim e^{\pm\pi a/2}$).

An efficient method to compute the coefficients was described in Gil et al. [2002a] and Temme [1975]; this method is based on the fact that both f_k and r_k satisfy the three-term recurrence relation

$$(k^2 + a^2)r_k - (2k-1)r_{k-1} + r_{k-2} = 0. \tag{6}$$

Perron's theorem is inconclusive with respect to the existence of minimal solutions for this recurrence relation; anyhow, the second equation in (6) confirms that neither f_k nor r_k are minimal solutions. Therefore, forward recursion will be numerically stable. Starting values can be computed taking into account that $\arg\Gamma(1+ia) = \sigma_0(a)$, where $\sigma_0(a)$ is the Coulomb phase shift, for which Chebyshev expansions are available for double precision [Cody and Hillstrom 1970]. Namely, we have:

$$\begin{aligned} r_0 &= \cos[\sigma_0(a) - a\ln(x/2)], \\ r_1 &= \frac{1}{1+a^2}\{\cos[\sigma_0(a) - a\ln(x/2)] - a\sin[\sigma_0(a) - a\ln(x/2)]\}, \end{aligned} \tag{7}$$

and

$$
\begin{aligned}
f_0 &= \frac{1}{a}\sin[\sigma_0(a) - a\ln(x/2)], \\
f_1 &= \frac{1}{a(1+a^2)}\{\sin[\sigma_0(a) - a\ln(x/2)] + a\cos[\sigma_0(a) - a\ln(x/2)]\}.
\end{aligned}
\tag{8}
$$

These formulas correct two misprints in [Gil et al. 2002a, Eqs. 12 and 13].

Series can be used for x/a small. See Gil et al. [2004], Section 2 .

2.2 Asymptotic Expansions for Large x

Asymptotic expansions for large x are available from the known asymptotic expansion of $I_\nu(x)$ [Abramowitz and Stegun 1964, Eq. 9.7.1]:

$$
\begin{aligned}
K_{ia}(x) &= \left(\frac{\pi}{2x}\right)^{1/2} e^{-x}\left\{\sum_{k=0}^{n-1}\frac{(ia,k)}{(2x)^k} + \gamma_n\right\}, \\
L_{ia}(x) &= \frac{1}{\sqrt{2\pi x}}e^{x}\left\{\sum_{k=0}^{n-1}(-1)^k\frac{(ia,k)}{(2x)^k} + \delta_n\right\},
\end{aligned}
\tag{9}
$$

where (ia, m) is the Hankel symbol, which satisfies

$$
(ia, k+1) = -\frac{\left(k+\frac{1}{2}\right)^2 + a^2}{k+1}(ia,k), \quad (ia,0) = 1. \tag{10}
$$

Bounds for the error terms (γ_n, δ_n) can be found in [Olver 1997, Pg. 269, Ex. 13.2].

As discussed in Gil et al. [2002a] the numerical performance of the asymptotic expansion for $K_{ia}(x)$ is of more restricted applicability than for the case of the evaluation of $K_\nu(x)$ for real ν. Furthermore, the continued fraction method described in Gil et al. [2002a] covers the region where this expansion is of numerical interest. For this reason, the continued fraction method is the preferred algorithm for the evaluation of $K_{ia}(x)$ and $K'_{ia}(x)$ for moderate values of a. On the other hand the asymptotic expansion for $L_{ia}(x)$ turns out to be accurate in a wider region, which is a fortunate situation given that the continued fraction method is not available in this case. See Gil et al. [2004], Section 2, for further details.

Asymptotic expansions for the derivatives are also available by differentiating Equations (9).

2.3 Airy-Type Uniform Asymptotic Expansions

The Airy-type asymptotic expansions for $K_{ia}(x)$ can be found in Balogh [1967] and Dunster [1990] and Olver [1997, pg. 425]; the analogous expansions for $L_{ia}(x)$ [Dunster 1990] and $K'_{ia}(x)$ are also available [Balogh 1967], while the expansion for $L'_{ia}(x)$ can be derived in the same way. We summarize here the main features needed for the computation through these expansions, neglecting the error terms. Further details can be found in Balogh [1967], Dunster [1990], Olver [1997], Gil et al. [2003], and Temme [1997].

The expansion for $K_{ia}(x)$ and $L_{ia}(x)$ in terms of Airy functions (Ai(z), Bi(z) and their derivatives) reads

$$
\begin{aligned}
K_{ia}(az) &= \frac{\pi e^{-a\pi/2}\phi(\zeta)}{a^{1/3}}\left[\mathrm{Ai}(-a^{2/3}\zeta)F_a(\zeta)+\frac{1}{a^{4/3}}\mathrm{Ai}'(-a^{2/3}\zeta)G_a(\zeta)\right],\\
L_{ia}(az) &= \frac{e^{a\pi/2}\phi(\zeta)}{2a^{1/3}}\left[\mathrm{Bi}(-a^{2/3}\zeta)F_a(\zeta)+\frac{1}{a^{4/3}}\mathrm{Bi}'(-a^{2/3}\zeta)G_a(\zeta)\right],
\end{aligned}
\tag{11}
$$

where

$$
F_a(\zeta)\sim\sum_{s=0}^{\infty}(-)^s\frac{a_s(\zeta)}{a^{2s}},\quad G_a(\zeta)\sim\sum_{s=0}^{\infty}(-)^s\frac{b_s(\zeta)}{a^{2s}},
\tag{12}
$$

as $a\to\infty$ uniformly with respect to $z\in[0,\infty)$. Error bounds for the asymptotic expansions of the $K_{ia}(x)$ and $L_{ia}(x)$ are given in Dunster [1990].

The quantity ζ is given by

$$
\begin{aligned}
\tfrac{2}{3}\zeta^{3/2} &= \log\frac{1+\sqrt{1-z^2}}{z}-\sqrt{1-z^2},\quad 0\le z\le 1,\\
\tfrac{2}{3}(-\zeta)^{3/2} &= \sqrt{z^2-1}-\arccos\frac{1}{z},\quad z\ge 1,
\end{aligned}
\tag{13}
$$

and

$$
\phi(\zeta)=\left(\frac{4\zeta}{1-z^2}\right)^{1/4},\quad \phi(0)=2^{1/3}.
\tag{14}
$$

Of course, it is crucial to accurately compute Equations (13) for small ζ. For this, series expansions around $z=1$ can be used.

The evaluation of the coefficients near the turning point $z=1$ (which is our region of interest) can be performed via Maclaurin series expansions of the quantities ϕ, a_s and b_s([Temme 1997]) in terms of the variable $\eta=2^{-1/3}\zeta$ (see Gil et al. [2003] and Temme [1997] for further details).

Asymptotic expansions for the derivatives can be found by differentiating Equations (11). In this way:

$$
\begin{aligned}
K'_{ia}(az) &= 2\frac{\pi e^{-a\pi/2}}{za^{2/3}\phi(\zeta)}\left[\mathrm{Ai}'(-a^{2/3}\zeta)P_a(\zeta)+\frac{1}{a^{2/3}}\mathrm{Ai}(-a^{2/3}\zeta)Q_a(\zeta)\right],\\
L'_{ia}(az) &= \frac{e^{a\pi/2}}{za^{2/3}\phi(\zeta)}\left[\mathrm{Bi}'(-a^{2/3}\zeta)P_a(\zeta)+\frac{1}{a^{2/3}}\mathrm{Bi}(-a^{2/3}\zeta)Q_a(\zeta)\right],
\end{aligned}
\tag{15}
$$

where $P_a(\zeta)$ and $Q_a(\zeta)$ can be written in terms of $F_a(\zeta)$, $G_a(\zeta)$ and their derivatives and they have asymptotic expansions

$$
P_a(\zeta)\sim\sum_{s=0}^{\infty}(-)^s\frac{c_s(\zeta)}{a^{2s}},\quad Q_a(\zeta)\sim\sum_{s=0}^{\infty}(-)^s\frac{d_s(\zeta)}{a^{2s}},
\tag{16}
$$

whose coefficients can be obtained from the computed coefficients a_s and b_s (in Taylor series around $\zeta = 0$) through the relations:

$$\begin{aligned} c_s(\zeta) &= a_s(\zeta) + \chi(\zeta) b_{s-1}(\zeta) + b'_{s-1}(\zeta), \\ d_s(\zeta) &= -\chi(\zeta) a_s(\zeta) - a'_s(\zeta) - \zeta b_s(\zeta), \end{aligned} \tag{17}$$

where

$$\chi(\zeta) = \phi'(\zeta)/\phi(\zeta), \tag{18}$$

The prime in Equations (17) and (18) denotes the derivative with respect to ζ. Using Equations (17) the coefficients c_s and d_s can be computed from the coefficients a_s and b_s. Details on the evaluation of a_s and b_s are given in Gil et al. [2003], where an explicit Maple algorithm is given for the computation of a_s and b_s for $s = 0, 1, 2, 3$.

By computing the Wronskian relation for the modified Bessel functions and using the Wronskian for Bessel functions, it is easy to derive the relation

$$F_a(\zeta) P_a(\zeta) - \frac{1}{a^2} G_a(\zeta) Q_a(\zeta) = 1, \tag{19}$$

which is a useful relation for checking the correctness of the approximations for the coefficients in the asymptotic expansions.

An algorithm to compute Airy functions of a real variable is needed for the computation of these asymptotic expansions. In the routines Gil et al. [2004] we use Algorithm 819 [Gil et al. 2002b].

These Airy-type asymptotic expansion are applied in Gil et al. [2004] in a broad region around the turning point line $a = x$.

2.4 Non-Oscillating Integral Representations

Paths of steepest descent for integral representations of the modified Bessel functions of imaginary orders and their derivatives are given in Temme [1994]. Apart from their application in asymptotics [Fabijonas 2002], these integrals are useful for building numerically stable (non-oscillating) integral representations for $K_{ia}(x)$ and $K'_{ia}(x)$, as described in Gil et al. [2002a]. We complete here the analysis in Gil et al. [2002a] by providing analogous expressions for the computation of $L_{ia}(x)$ and $L'_{ia}(x)$. Additionally, we study further transformations of the integrals that enable us to obtain integral expressions suitable for computation by means of the trapezoidal rule.

2.4.1 *Monotonic Case ($x > a$).* We have the following integral representations in the monotonic region Gil et al. [2002a]

$$\begin{aligned} K_{ia}(x) &= e^{-\lambda} \int_0^\infty e^{-x\Phi(\tau)} d\tau \\ K'_{ia}(x) &= -e^{-\lambda} \int_0^\infty \left[\cos\theta + \frac{\cosh\tau - 1 + 2\sin^2 \frac{1}{2}(\theta - \sigma)}{\cos\sigma} \right] e^{-x\Phi(\tau)} d\tau, \end{aligned} \tag{20}$$

where

$$\lambda = x\cos\theta + a\theta\,,\ a = x\sin\theta\,,\ \sin\sigma = \left(\sin\theta\frac{\tau}{\sinh\tau}\right) \tag{21}$$

and $\theta \in [0, \pi/2)$, $\sigma \in (0, \theta]$. The dominant exponential term ($e^{-\lambda}$) has been factored out. The argument of the exponential in the integrand is

$$\Phi(\tau) = (\cosh\tau - 1)\cos\sigma + 2\sin\left(\frac{\theta-\sigma}{2}\right)\sin\left(\frac{\theta+\sigma}{2}\right) + (\sigma-\theta)\sin\theta\,. \tag{22}$$

This formula corrects a misprint in Gil et al. [2002a] (Eq. 33). The difference $\theta-\sigma$ can be computed in a stable way for small values of τ by using the expression.

$$\sin(\theta-\sigma) = \frac{\sin\theta}{\cos\theta\dfrac{\tau}{\sinh\tau} + \cos\sigma}\left[1 - \frac{\tau^2}{\sinh^2\tau}\right], \tag{23}$$

together with the definition of σ (21) and specific algorithms to compute $\cosh(\tau) - 1$ and $1 - \sinh(\tau)^2/\tau^2$ for small τ.

The non-oscillating integral representations for $L_{ia}(x)$ and its derivative can be written after factoring the dominant exponential contribution as:

$$L_{ia}(x) = \frac{e^{\lambda}}{2\pi}\left[\int_{-\theta-\pi}^{-\theta+\pi} e^{x\gamma(\sigma)}d\sigma - (1-e^{-2\pi a})e^{-\eta}\int_0^{+\infty} e^{-x\Phi(\tau)}\frac{d\sigma}{d\tau}d\tau\right] \tag{24}$$

where

$$\begin{aligned}\gamma(\sigma) &= 2\sin\frac{\theta-\sigma}{2}\sin\frac{\theta+\sigma}{2} + (\sigma-\theta)\sin\theta\\ \eta &= 2x[\cos\theta + (\theta-\pi/2)\sin\theta] = 2x\left(\sqrt{1-(a/x)^2} - \tfrac{a}{x}\arccos(\tfrac{a}{x})\right)\end{aligned} \tag{25}$$

and using Eq. (21)

$$\frac{d\sigma}{d\tau} = \tan\sigma\left[\frac{1}{\tau} - \coth\tau\right]. \tag{26}$$

The first integral is dominant over the second one for large values of the parameters and a/x not too close to $a = x$. As $a \to x$ both integrals become of the same order.

Similarly, we have the following representation for $L'_{ia}(x)$:

$$L'_{ia}(x) = \frac{e^{\lambda}}{2\pi}\left[\int_{-\theta-\pi}^{-\theta+\pi} \cos\sigma e^{x\gamma(\sigma)}d\sigma + (1-e^{-2\pi a})e^{-\eta}\int_0^{+\infty} e^{-x\Phi(\tau)}h(\tau)d\tau\right] \tag{27}$$

where

$$h(\tau) = \sin\sigma\left[\frac{\cosh\tau}{\tau} - \frac{1}{\sinh\tau}\right]. \tag{28}$$

These integral representations for $L_{ia}(x)$ and $L'_{ia}(x)$ can be used for checking the computation of these functions in the monotonic region. They are not used by our algorithms [Gil et al. 2004] because the Airy-type asymptotic expansion (Section 2.3) and the expansion for large x (Section 2.2) are sufficiently accurate for this functions and they are faster to compute (see Gil et al. [2004], Section 2).

2.4.2 *Oscillatory Case ($x < a$).* The non-oscillating integral representations for the oscillatory region are more difficult to evaluate numerically than those for the monotonic case. Indeed, as it was discussed in Gil et al. [2002a], the steepest descent method leads to three integrals, which have to be computed separately. However, as we later discuss, for moderately large a it will be enough to compute a single integral.

In Gil et al. [2002a], the following formula was obtained:

$$
\begin{aligned}
K_{ia}(x) = e^{-\pi a/2}\Bigg[& \int_{\mu}^{\infty} e^{-\Psi(\tau)}\left(\cos\chi + \sin\chi\frac{d\sigma}{d\tau}\right)d\tau \\
& + \frac{1}{\sinh \pi a}\int_{\mu-\tanh\mu}^{\mu}\left(\cos\chi\,\sinh\rho + \sin\chi\,\cosh\rho\,\frac{d\sigma}{d\tau}\right)d\tau \\
& - \frac{1}{\sinh \pi a}\int_{\pi}^{3\pi/2}\left(\cos\chi\,\sinh\rho\,\frac{d\tau}{d\sigma} + \sin\chi\,\cosh\rho\right)d\sigma\Bigg],
\end{aligned}
\tag{29}
$$

where $\chi = x\sinh\mu - a\mu$, $\cosh\mu = \frac{a}{x}$, $\mu > 0$,

$$
\Psi(\tau) = x\cosh\tau\,\cos\sigma + a\left(\sigma - \frac{1}{2}\pi\right), \rho(\tau) = -\Psi(\tau) + a\pi \tag{30}
$$

and

$$
\sin\sigma = \frac{(\tau-\mu)\cosh\mu + \sinh\mu}{\sinh\tau}. \tag{31}
$$

Notice that each of the three integrals in Eq. (29) can in principle be integrated with respect to either of the variables σ and τ, taking into account Eq. (31) together with the fact that the integration path $\tau(\sigma)$ is such that $\tau(0) = +\infty$, $\tau(\pi/2) = \mu$, $\tau(\pi) = \mu - \tanh\mu > \tau(3\pi/2)$; however, as discussed in Gil et al. [2002a] there are strong numerical reasons for the selections made. In particular, the third integral is performed with respect to σ (which requires numerical inversion of (31)) to avoid the singularity of $d\sigma/d\tau$ at $\tau(3\pi/2)$. As explained in Gil et al. [2002a] the numerical inversion of (31) in the interval $\sigma \in [\pi, 3\pi/2]$ can be efficiently performed in parallel with the numerical integration.

Similar integral representations exist for $K'_{ia}(x)$, $L_{ia}(x)$ and $L'_{ia}(x)$. We have:

$$
\begin{aligned}
K'_{ia}(x) = e^{-\pi a/2}\Bigg[& \int_{\mu}^{\infty} e^{-\Psi(\tau)}\left(\cos\chi\,A(\tau) + \sin\chi\,C(\tau)\right)d\tau \\
& + \frac{1}{\sinh \pi a}\int_{\mu-\tanh\mu}^{\mu}\left(\cos\chi\,\cosh\rho\,A(\tau) + \sin\chi\,\sinh\rho\,C(\tau)\right)d\tau \\
& - \frac{1}{\sinh \pi a}\int_{\pi}^{3\pi/2}\left(\cos\chi\,\cosh\rho\,B(\tau(\sigma)) + \sin\chi\,\sinh\rho\,D(\tau(\sigma))\right)d\sigma\Bigg]
\end{aligned}
\tag{32}
$$

where

$$
\begin{aligned}
A(\tau) &= -\cosh\tau\cos\sigma + \sinh\tau\sin\sigma\frac{d\sigma}{d\tau}, \quad B(\tau) = A(\tau)\frac{d\tau}{d\sigma}, \\
C(\tau) &= -\sinh\tau\sin\sigma - \cosh\tau\cos\sigma\frac{d\sigma}{d\tau}, \quad D(\tau) = C(\tau)\frac{d\tau}{d\sigma}.
\end{aligned}
\tag{33}
$$

In addition, integral representations for $L_{ia}(x)$ and its derivative are:

$$
\begin{aligned}
L_{ia}(x) = \frac{e^{\pi a/2}}{\pi}\Bigg[& \frac{1-e^{-2\pi a}}{2}\int_{\mu}^{\infty} e^{-\Psi(\tau)}\left(\sin\chi - \cos\chi \frac{d\sigma}{d\tau}\right) d\tau \\
& + e^{-\pi a}\int_{\mu-\tanh\mu}^{\mu}\left(\sin\chi\,\sinh\rho - \cos\chi\,\cosh\rho\,\frac{d\sigma}{d\tau}\right) d\tau \\
& - e^{-\pi a}\int_{\pi}^{3\pi/2}\left(\sin\chi\,\sinh\rho\,\frac{d\tau}{d\sigma} - \cos\chi\,\cosh\rho\right) d\sigma \Bigg]
\end{aligned} \tag{34}
$$

and

$$
\begin{aligned}
L'_{ia}(x) = \frac{e^{\pi a/2}}{\pi}\Bigg[& \frac{1-e^{-2\pi a}}{2}\int_{\mu}^{\infty} e^{-\Psi(\tau)}\left(\sin\chi\, A(\tau) - \cos\chi\, C(\tau)\right) d\tau \\
& + e^{-\pi a}\int_{\mu-\tanh\mu}^{\mu}\left(\sin\chi\,\cosh\rho\, A(\tau) - \cos\chi\,\sinh\rho\, C(\tau)\right) d\tau \\
& - e^{-\pi a}\int_{\pi}^{3\pi/2}\left(\sin\chi\,\cosh\rho\, B(\tau(\sigma)) - \cos\chi\,\sinh\rho\, D(\tau(\sigma))\right) d\sigma \Bigg].
\end{aligned} \tag{35}
$$

Notice that the dominant exponential behaviour has been factored for both the functions $K_{ia}(x)$ and $L_{ia}(x)$ and their derivatives, which coincides with the exponential behaviour of the uniform asymptotic expansion. This is an interesting feature when computing scaled functions in order to avoid overflows and/or underflows in the computation. After factoring the dominant exponential terms ($e^{\pm\pi a/2}$), the overflow and/or underflow problems are eliminated; notice, however, that when computing the integrals over finite intervals we should evaluate $\sinh(\rho)/e^{a\pi}$, $\cosh(\rho)/e^{a\pi}$ for $L_{ia}(x)$ and its derivative and $\sinh(\rho)/\sinh a\pi$, $\cosh(\rho)/\sinh a\pi$ for $K_{ia}(x)$ (and $K'_{ia}(x)$) instead of computing the hyperbolic and the exponential separately (otherwise, overflows will take place for moderately large a). For this reason it is convenient to use the expressions

$$
\frac{\cosh\rho}{\sinh\pi a} = e^{-\psi}\frac{1+e^{-2\rho}}{1-e^{-2\pi a}}, \quad \frac{\sinh\rho}{\sinh\pi a} = e^{-\psi}\frac{1-e^{-2\rho}}{1-e^{-2\pi a}} \tag{36}
$$

in the evaluation of Equations (29) and (32) and to proceed in the same way for $e^{-\pi a}\cosh\rho$ and $e^{-\pi a}\sinh\rho$ in Equations (34) and (35). Notice that in the oscillatory region $\rho > 0$ and that for large a and x both $e^{-2\rho}$ and $e^{-2\pi a}$ will underflow. These underflow problems can be easily avoided by neglecting these exponential terms for large parameters.

In addition, when both exponentials become negligible, the integral over sigma becomes negligible and the remaining two integrals can be approximated by only one integral. We can write

$$
\begin{aligned}
K_{ia}(x) &\approx e^{-\pi a/2}\left[\int_{\tau_0}^{\infty} e^{-\Psi(\tau)}\left(\cos\chi + \sin\chi\frac{d\sigma}{d\tau}\right)d\tau + \mathcal{O}(e^{-\pi a/2})\right]\\
K'_{ia}(x) &\approx e^{-\pi a/2}\left[\int_{\tau_0}^{\infty} e^{-\Psi(\tau)}\left(\cos\chi\, A(\tau) + \sin\chi\, C(\tau)\right)d\tau + \mathcal{O}(e^{-\pi a/2})\right]\\
L_{ia}(x) &\approx \frac{e^{\pi a/2}}{2\pi}\left[\int_{\tau_0}^{\infty} e^{-\Psi(\tau)}\left(\sin\chi - \cos\chi\frac{d\sigma}{d\tau}\right)d\tau + \mathcal{O}(e^{-\pi a/2})\right]\\
L'_{ia}(x) &\approx \frac{e^{\pi a/2}}{2\pi}\left[\int_{\tau_0}^{\infty} e^{-\Psi(\tau)}\left(\sin\chi\, A(\tau) - \cos\chi\, C(\tau)\right)d\tau + \mathcal{O}(e^{-\pi a/2})\right]
\end{aligned}
\tag{37}
$$

where

$$\tau_0 = \mu - \tanh\mu.$$

These approximations can be used for moderately large a, which is the region where integrals for the oscillatory case are employed in the code [Gil et al. 2004].

It is useful however to have the complete expressions for testing the rest of the methods. The computation through quadrature using Equations (20), (24), (27), (29), (32), (34) and (35), provides a way for computing the functions in the whole (x, a) plane, except close to $a = x$, where the integrands become nonsmooth. For this reason, they have been used for checking the algorithm, although in the oscillatory region only Equation (37) is necessary when building the numerical algorithm [Gil et al. 2004].

2.4.3 *Quadrature Rule.* As reported in Goodwin [1949], the trapezoidal rule is a very efficient method of computation of integrals $\int_{-\infty}^{+\infty} f(x)dx$ for rapidly decaying integrands $f(x)$; in particular, it is know that the error decays as $\exp(-(\pi/h)^2)$ for integrals of the type $\int_{-\infty}^{+\infty} e^{-x^2} g(x)dx$ with g analytic in $\{z \in \mathbb{C} : |\Im z| < \pi/h\}$. After appropriate changes of variable, similar arguments follow for integrals over finite intervals with a smooth integrand [Schwarz 1969; Takahasi and Mori 1973, 1974].

The semi-infinite integrals in this Section are appropriate for their computation by using the trapezoidal rule, because they decay as a double exponential as $\tau \to +\infty$. On the other hand, the integrals over finite intervals show abrupt variations as $a \to x$, particularly in the oscillatory case, but under an adequate change of variables they can be also computed efficiently by means of the trapezoidal rule. For finite integrals, we consider a change of variable in order to map the finite interval $[a, b]$ into $(-\infty, +\infty)$ and a successive change to improve the convergence of the trapezoidal rule [Takahasi and Mori 1973, 1974]; namely, we consider the following transformation:

$$
\begin{aligned}
I &= \int_a^b f(x)dx = \int_{-\infty}^{+\infty} g(t)dt\,,\ \ g(t) = f(x(t))\frac{(b-a)\cosh t}{2\cosh^2(\sinh t)},\\
x(t) &= \frac{b+a}{2} + \frac{b-a}{2}\tanh(\sinh t).
\end{aligned}
\tag{38}
$$

And the integral is discretized by means of the trapezoidal rule with equal mesh size:

$$\int_{-\infty}^{+\infty} g(t)dt = h \sum_{n=-\infty}^{+\infty} g(nh) + \epsilon, \tag{39}$$

where the error ϵ is expected to decay very quickly as the mesh size is decreased because the integrand is analytic and its decay is doubly exponential. We use a trapezoidal rule that halves the mesh size until the prescribed precision is reached; the same rule controls that the truncation of the infinite series (39) gives an error well below the accuracy claim.

Regarding the semi-infinite integrals, we use a change of variable to transform the integration interval $[a, +\infty)$ to $(-\infty, \infty)$. We consider the following change of variables to perform this map.

$$\tau(x) = a + \sinh^{-1}(e^x). \tag{40}$$

The additional change $x = \sinh t$ improves the convergence of the trapezoidal rule.

It is observed that, typically, no more than 8 iterations of the trapezoidal rule are needed, which means that the integrands are evaluated at $2^8 + 1 = 257$ points in the worst cases. This is the typical number of iterations for the evaluation of $\int_{-\infty}^{+\infty} e^{-x^2} dx$ by means of a recursive trapezoidal rule when double precision accuracy is demanded. This fact confirms that the above mentioned changes of variable are adequate for the computation of the integrals for the modified Bessel functions.

2.5 Continued Fraction Method

As discussed in Gil et al. [2002a] both $K_{ia}(x)$ and K'_{ia} can be computed for moderate a by means of a continued fraction method, similar to the corresponding method for Bessel functions of real orders (see Temme [1975] and [Press et al. 1992, pp. 239–240]). We refer to Gil et al. [2002a] for a full description of this scheme.

As numerical experiments show, this method is competitive in speed with asymptotic expansions for large x (Section 2.2) and the range of application is larger. Therefore, the continued fraction method substitutes the use of asymptotic expansions for large x.

3. RANGE OF COMPUTATION AND SCALED FUNCTIONS

As described in previous sections, the integral representations that were developed indicate that the dominant behaviour for the functions when the parameters are large is of exponential type. This means that the computations can only be carried for not too large values of a and x in order to avoid overflows/underflows in the computation. For instance, from Equations (29) and (32) it is seen that for large a ($a > x$), we have $K_{ia}(x) \sim e^{-a\pi/2}$ and similarly for the derivative, while for $L_{ia}(x)$ and its derivative (Equations (34) and (35)) the asymptotic behaviour is $\sim e^{a\pi/2}$. This means that to avoid overflow/underflows

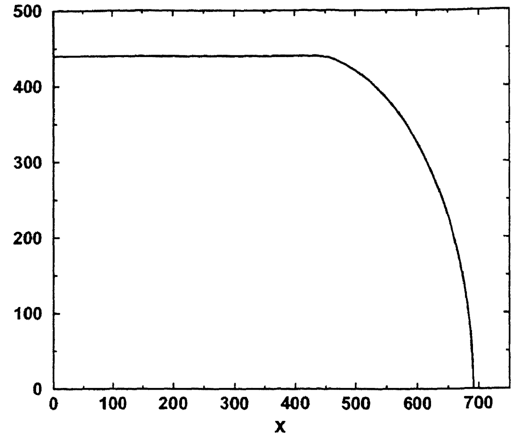

Fig. 1. Computable range for the evaluation of $K_{ia}(x)$, $L_{ia}(x)$ and their derivatives.

in the computation, we must restrict the range of a in the oscillatory region to

$$a < 2\ln(10^n N)/\pi \tag{41}$$

where N is either the inverse of the underflow number (when computing $K_{ia}(x)$ or its derivative) or the overflow number (for $L_{ia}(x)$ and its derivative); 10^n is a safety factor (in the program, we take $n = 8$). For processors using the IEEE standard in double precision this will approximately limit a to $a < 440$. On the other hand, for the monotonic region ($x > a$) the integral representations show that the dominant exponential behaviour is $K_{ia}(x) \sim e^{-\lambda}$, $L_{ia}(x) \sim e^{+\lambda}$ where $\lambda(x,a) = x(\cos\theta + \theta\sin\theta)$, $\sin\theta = a/x$ ($\theta \in [0, \pi/2]$), and similarly for the derivatives. This means that, in order to avoid overflows/underflows, the range of computation must be restricted to:

$$\lambda(a,x) = \sqrt{x^2 - a^2} + a\ \arcsin(a/x) < \ln(10^n N)\,. \tag{42}$$

Figure 1 shows the computable range for $10^n N = 10^{300}$ (typical value for IEEE standard double precision)

Given that all our expressions have the dominant exponential contributions factored out, exponentially scaled functions can be defined that are computable in wider ranges. Namely, we define:

$$\widetilde{K_{ia}}(x) = \begin{cases} e^{\lambda(x,a)} K_{ia}(x) & x \geq a \\ e^{a\pi/2} K_{ia}(x) & x < a \end{cases} \qquad \widetilde{K'_{ia}}(x) = \begin{cases} e^{\lambda(x,a)} K'_{ia}(x) & x \geq a \\ e^{a\pi/2} K'_{ia}(x) & x < a \end{cases} \tag{43}$$

and

$$\widetilde{L_{ia}}(x) = \begin{cases} e^{-\lambda(x,a)} L_{ia}(x) & x \geq a \\ e^{-a\pi/2} L_{ia}(x) & x < a \end{cases} \qquad \widetilde{L'_{ia}}(x) = \begin{cases} e^{-\lambda(x,a)} L'_{ia}(x) & x \geq a \\ e^{-a\pi/2} L'_{ia}(x) & x < a. \end{cases} \tag{44}$$

Note that, as in the rest of the article, we are considering positive a because $K_{ia}(x)$ and $L_{ia}(x)$ are even functions of a. Of course, when applying the scaling factors for negative a, we should replace a by $|a|$ in the exponential scaling factors of Equations (43) and (44). In this way, the scaled functions are also even functions of a.

The definitions in (43) and (44) eliminate exactly the front exponential factor in the oscillatory region ($a > x$) from the series and the Airy type asymptotic expansion and in all the (x, a) plane for the the integral representations. In other cases, there remains an exponential factor with soft variation. For example, when using Airy-type expansions in the monotonic region (neglecting non-exponential factors), we have

$$\widetilde{K_{ia}}(x) \sim e^{\lambda - a\pi/2} = e^{\tilde{\lambda}} \tag{45}$$

where

$$\tilde{\lambda} = x(\cos\theta + (\theta - \pi/2)\sin\theta) = \sqrt{x^2 - a^2} + a(\arcsin(a/x) - \pi/2),$$

which is small for $x \simeq a$ ($\theta \simeq \pi/2$); loss of accuracy in the computation of $\tilde{\lambda}$ for $x \simeq a$ can be reduced by expanding $\tilde{\lambda}$ in powers of $\theta - \pi/2$.

Similarly, an exponential factor remains when rescaling the asymptotic expansions and the same happens when applying the continued fraction method. In this case, we have for $x > a$;

$$\widetilde{K_{ia}}(x) \sim e^{x-\lambda} = e^{-\bar{\lambda}} \tag{46}$$

where

$$\bar{\lambda} = x((\cos\theta - 1) + \theta\sin\theta) = x - \sqrt{x^2 - a^2} - a\ \arcsin(a/x),$$

which goes to zero as $a/x \to 0$ ($\theta \to 0$). Loss of accuracy in the computation of $\bar{\lambda}$ for small θ (a/x small) can be avoided by expanding $\bar{\lambda}$ in powers of θ.

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