Algorithm 822: GIZ, HIZ: Two Fortran 77 Routines for the Computation of Complex Scorer Functions

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Two Fortran 77 routines for the evaluation of Scorer functions of complex arguments Gi(z), Hi(z), and their derivatives are presented. The routines are based on the use of quadrature, Maclaurin series, and asymptotic expansions. For real z, comparison with a previous code by A. J. MacLeod [1994] is provided.

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1. INTRODUCTION

This algorithm computes the Scorer functions Gi(z) and Hi(z) in the complex plane. Scorer functions are solutions of the inhomogeneous Airy differential equations

$$\begin{aligned} \mathrm{Gi}'' - z\mathrm{Gi} &= -\frac{1}{\pi}, \\ \mathrm{Hi}'' - z\mathrm{Hi} &= \frac{1}{\pi}, \end{aligned} \tag{1}$$

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with initial values

$$\begin{aligned} \mathrm{Gi}(0) &= \frac{1}{2}\mathrm{Hi}(0) = \frac{1}{3}\mathrm{Bi}(0) = \frac{1}{\sqrt{3}}\mathrm{Ai}(0) = \frac{1}{3^{7/6}\Gamma(2/3)}, \\ \mathrm{Gi}'(0) &= \frac{1}{2}\mathrm{Hi}'(0) = \frac{1}{3}\mathrm{Bi}'(0) = -\frac{1}{\sqrt{3}}\mathrm{Ai}'(0) = \frac{1}{3^{5/6}\Gamma(1/3)}. \end{aligned} \tag{2}$$

Because Scorer functions and Airy functions solve the inhomogeneous equation $w'' - zw = K$, with K constant, Scorer functions appear in asymptotic expansions for inhomogeneous equations around a turning point [Olver 1997, P. 429]. Scorer functions appear in a number of applications in physics and chemistry (see, e.g., Lee [1980], MacLeod [1994], and Sakharov and Tereschenko [1996] for real variables and Romalis and Happer [1999] for complex variables).

Properties of the Scorer functions are given in Chapter 10 of Abramowitz and Stegun [1964]. In Gil et al. [2001] stable integral representations of the Scorer functions have been derived, with a discussion of methods for numerical quadrature. Relevant properties and conclusions from our earlier paper are given in the next section.

For the evaluation of real argument Scorer functions, 20D coefficients of Chebyshev expansions for Gi and Hi are given in MacLeod [1994]. For complex argument no published algorithms seem to be available. We provide an algorithm, based on Maclaurin series for small $|z|$, quadrature for intermediate values, and asymptotic expansions for large $|z|$. In the algorithm we also use values of the Airy function $\mathrm{Ai}(z)$ and $\mathrm{Bi}(z)$, which are computed by algorithms given in Gil et al. [2002b].

The program gives the option of computing scaled Scorer functions in order to enlarge the range of computation in the sectors of the complex plane where the functions become exponentially large for large $|z|$.

The relative accuracy for the modulus of the functions is better than 10^{-12}, except, of course, near their zeros, where the accuracy must be interpreted as absolute accuracy. Regarding the computation of the phase of the functions, 10^{-12} is the absolute accuracy. See Gil et al. [2002b] for further comments on the accuracy claims when computing functions in the complex plane in finite precision arithmetic.

The accuracy of the codes is limited by the accuracy in the computation of the Airy functions $\mathrm{Ai}(z)$ and $\mathrm{Bi}(z)$ in the sectors of the complex plane where connection formulas (4), (6), and (5) are used. Given that the codes in Gil et al. [2002b] provide an accuracy better than 10^{-13}, a conservative claim for Scorer functions is that the accuracy is better than 10^{-12} (the accuracy for $\mathrm{Hi}(z)$ is better in the sector where connection formulas are not used). Similarly to that described in Gil et al. [2002b], the accuracy in the computation of the unscaled Scorer functions $\mathrm{Hi}(z)$ and $\mathrm{Gi}(z)$ will gradually worsen as larger $|z|$ values ($|z| > 30$) are considered, particularly when relations involving Airy functions are required (Equations (4) to (6)) and Airy functions are dominant for large z. This degradation in accuracy is eliminated by scaling the functions in these sectors (see Section 2.2). Similarly as for Airy functions, there is a case for which not even scaling avoids the accuracy degradation: relative accuracy in the computation of $\mathrm{Gi}(z)$ on the negative real axis is gradually lost as larger $|z|$ is considered, and this degradation is similar to that described in Gil et al. [2002b] (because $\mathrm{Gi}(-x) \sim \mathrm{Bi}(-x)$ for large x).

2. METHOD OF COMPUTATION

We briefly summarize the results of Gil et al. [2001] and indicate the numerical methods for different regions in the complex plane.

Several symmetry rules and connection formulas are available for computing the Scorer functions. Some relations produce large numerical errors, because of cancellation, and these relations should be avoided. As explained in Gil et al. [2001], the direct evaluation of the function $\mathrm{Hi}(z)$ is needed in a certain sector in the complex plane; in the rest of the complex plane, stable connection formulas are available. Conjugation is used throughout.

We have the following stable schemes.

Scheme for $\mathrm{Hi}(z)$.

—If $\mathrm{ph}\, z \in [\frac{2}{3}\pi, \pi]$ then use quadrature of the representation

$$\mathrm{Hi}(z) = \frac{1}{\pi} \int_0^{\infty} e^{zt-(1/3)t^3}\, dt. \tag{3}$$

—If $\mathrm{ph}\, z \in [0, \frac{2}{3}\pi[$ then use the connection formula

$$\mathrm{Hi}(z) = e^{2\pi i/3}\mathrm{Hi}(ze^{2\pi i/3}) + 2e^{-\pi i/6}\mathrm{Ai}(ze^{-2\pi i/3}). \tag{4}$$

Scheme for $\mathrm{Gi}(z)$).

—If $\mathrm{ph}\, z \in [\frac{2}{3}\pi, \pi]$ then use the connection formula

$$\mathrm{Gi}(z) = \mathrm{Bi}(z) - \mathrm{Hi}(z). \tag{5}$$

—If $\mathrm{ph}\, z \in [0, \frac{2}{3}\pi[$ then use the connection formula

$$\mathrm{Gi}(z) = -e^{2\pi i/3}\mathrm{Hi}(ze^{2\pi i/3}) + i\mathrm{Ai}(z). \tag{6}$$

These schemes are slightly different from the ones in Gil et al. [2001]. The connection formula (6) is not given in Gil et al. [2001], but follows from combining (2.7) and (2.8); see also (3.17). The quadrature rule is used in the sector where $\mathrm{Hi}(z)$ is of order $\mathcal{O}(1/z)$ for large z; see (13). In other sectors the Scorer functions may become exponentially large at infinity, and these cases are governed by the connection formulas with the Airy functions.

The method of computation of the derivatives, $\mathrm{Gi}'(z)$ and $\mathrm{Hi}'(z)$, consists of taking the derivative of Equations (3) to (5). For instance, taking the derivative with respect to z in Equation (3) we have:

$$\mathrm{Hi}'(z) = \frac{1}{\pi} \int_0^{\infty} t e^{zt-(1/3)t^3}\, dt, \tag{7}$$

which can be computed considering the same method we next describe for the computation of $\mathrm{Hi}(z)$.

In Gil et al. [2001], it was discussed how to compute the integral for Hi in (3) in a numerically stable way by properly deforming the integration path in order to avoid oscillations of the integrand. We write

$$z = x + iy, \qquad t = u + iv, \qquad \phi(t) = \frac{1}{3}t^3 - zt = \phi_r(u,v) + i\phi_i(u,v),$$

where

$$\phi_r(u,v) = \frac{1}{3}u^3 - uv^2 - xu + yv, \qquad \phi_i(u,v) = u^2 v - \frac{1}{3}v^3 - xv - yu.$$

Then we integrate along the contour defined by $\phi_i(u,v) = 0$, which starts at the origin and runs into a valley of the integrand. We obtain

$$\mathrm{Hi}(z) = \frac{1}{\pi}\int_0^\infty e^{-\phi_r(u,v(u))} h(u)\,du, \tag{8}$$

where $v(u)$ is the solution of $\phi_i(u,v) = 0$, and

$$h(u) = 1 + i\frac{dv(u)}{du} = 1 + i\frac{2uv - y}{v^2 - u^2 + x}.$$

In this way the integral becomes nonoscillating. Near the upper boundary of the sector $\mathrm{ph}\, z \in [\frac{2}{3}\pi, \pi]$; that is, near the half-line $y = -x\sqrt{3}, x < 0$, the relation between v and u becomes singular. In this case, it is better to use a different relation. We use a simple relation that fits the exact solution of $\phi_i(u,v) = 0$ at $u = 0$ and at $u = \infty$ by writing

$$v(u) = -\frac{y}{x}\frac{u}{u^2+1}, \qquad \frac{dv(u)}{du} = -\frac{y}{x}\frac{1-u^2}{(u^2+1)^2}.$$

This gives

$$\mathrm{Hi}(z) = \frac{1}{\pi}\int_0^\infty e^{-\phi_r(u,v(u)) - i\phi_i(u,v(u))} h(u)\,du, \tag{9}$$

where again $h(u) = 1 + i dv(u)/du$ with the new expression for the derivative. Representation (9) has oscillations in the integrand, but these do not cause any difficulties in the quadrature. It is important that $v(u)$ fits the exact solution at $u = 0$ in order to reduce the number of oscillations for small u, where the main contributions to the integral come from; of course, choosing the same behavior at $u = \infty$ is also crucial to ensure that the oscillations at large u do not contribute significantly to the computation of the integral. In this way, the oscillations for small u are eliminated or reduced and the contributions for large u are negligible.

The integrals in (8) and (9) are of the form $\int_0^\infty f(u)\,du$, where f is analytic in a neighborhood of $[0, \infty)$. For large u we have $f(u) = \mathcal{O}(\exp(-\frac{1}{3}u^3))$; hence f is decreasing very fast at ∞.

By writing $u = \ln(1 + e^s)$ the integral is transformed into

$$\int_0^\infty f(u)du = \int_{-\infty}^\infty f\left(\ln(1+e^s)\right)\frac{e^s\,ds}{1+e^s}$$

and to improve convergence at $-\infty$ a further substitution $s = \sinh t$ is used. The trapezoidal rule is very efficient on this type of integrals of analytic functions; see Gil et al. [2002a].

2.1 Series Expansions

The quadrature method works for all complex z in the indicated sectors. For efficiency reasons, power series and asymptotic expansions are used when possible.

The functions Gi and Hi are entire functions. The power series for Hi follows easily from (3), and reads

$$\mathrm{Hi}(z) = \frac{1}{\pi}\sum_{k=0}^{\infty} h_k \frac{z^k}{k!}, \qquad h_k = \int_0^{\infty} t^k e^{-(1/3)t^3}\, dt = 3^{(1/3)(k-2)}\Gamma\left(\frac{k+1}{3}\right). \tag{10}$$

For Gi such a simple derivation is not available. However, by using (see (2.8) of Gil et al. [2001])

$$\mathrm{Gi}(z) = -\frac{1}{2}[e^{2\pi i/3}\mathrm{Hi}(ze^{2\pi i/3}) + e^{-2\pi i/3}\mathrm{Hi}(ze^{-2\pi i/3})], \tag{11}$$

it follows that

$$\mathrm{Gi}(z) = \frac{1}{\pi}\sum_{k=0}^{\infty} g_k \frac{z^k}{k!}, \qquad g_k = -h_k \cos\frac{2}{3}\pi(k+1). \tag{12}$$

The power series are used for $|z| \le 1.5$. For large z we have the asymptotic expansion:

$$\mathrm{Hi}(z) \sim -\frac{1}{\pi z}\left[1 + \frac{1}{z^3}\sum_{s=0}^{\infty}\frac{(3s+2)!}{s!(3z^3)^s}\right], \quad z \to \infty, \quad |\mathrm{ph}(-z)| \le \frac{2}{3}\pi - \delta, \tag{13}$$

δ being an arbitrary positive constant. We use this expansion for $|z| \ge 20$, and to avoid the boundary of the sector of validity we take $\mathrm{ph}\, z \in [\frac{2}{3}\pi, \pi]$. This corresponds to the first item in Scheme 1. An asymptotic expansion for Gi is also available:

$$\mathrm{Gi}(z) \sim -\frac{1}{\pi z}\left[1 + \frac{1}{z^3}\sum_{s=0}^{\infty}\frac{(3s+2)!}{s!(3z^3)^s}\right], \quad z \to \infty, \quad |\mathrm{ph}(z)| \le \frac{\pi}{3} - \delta. \tag{14}$$

We use this expansion for $|z| > 30$, $|\mathrm{ph} z| < \pi/3 - 0.3$.

2.2 Scaling the Functions

The scaling of the functions is relevant for $\mathrm{Hi}(z)$ in the sector $\mathrm{ph}\, z \in [-\frac{1}{3}\pi, \frac{1}{3}\pi]$, where the function increases exponentially for large $|z|$. The dominant factor in the asymptotic behavior is $\exp(\zeta)$ with $\zeta = \frac{2}{3}z^{3/2}$. In this case, we define the scaled function (see Equation (4)) by

$$\widetilde{\mathrm{Hi}}(z) \equiv e^{-(2/3)z^{3/2}}\mathrm{Hi}(z) = e^{2\pi i/3}e^{-(2/3)z^{3/2}}\mathrm{Hi}(ze^{2\pi i/3}) + 2e^{-\pi i/6}\widetilde{\mathrm{Ai}}(ze^{-2\pi i/3}), \tag{15}$$

where $\widetilde{\mathrm{Ai}}$ is the scaled Airy function, which is computed by the code AIZ [Gil et al. 2002b]. In the remaining part of the plane $\mathrm{Hi}(z)$ is of order $\mathcal{O}(1/z)$; see (13).

For Gi(z) the scaling is relevant when $\mathrm{ph}(-z) \in [-\frac{2}{3}\pi, \frac{2}{3}\pi]$. Connection formulas (6) and (5) give the possibility of rescaling Gi; defining $\widetilde{\mathrm{Gi}} = \exp(\zeta)\mathrm{Gi}$ we have:

$$\widetilde{\mathrm{Gi}}(z) = -e^{2\pi i/3}e^{(2/3)z^{3/2}}\mathrm{Hi}(ze^{2\pi i/3}) + i\widetilde{\mathrm{Ai}}(z) \quad \text{for } \pi/3 \le |\mathrm{ph} z| \le 2\pi/3,$$
$$\widetilde{\mathrm{Gi}}(z) = -e^{(2/3)z^{3/2}}\mathrm{Hi}(z) + \widetilde{\mathrm{Bi}}(z) \quad \text{for } 2\pi/3 < |\mathrm{ph} z| \le \pi, \tag{16}$$

where $\widetilde{\mathrm{Bi}}(z)$ is the scaled function computed by the code BIZ [Gil et al. 2002b].

3. DESCRIPTION OF THE ROUTINES

We now describe the inputs and outputs of the main routines for the computation of Hi(z) and Gi(z) (GIZ and HIZ, respectively).

The routine GIZ depends on HIZ, and both HIZ and GIZ call the external codes AIZ and BIZ for the computation of the complex Airy functions Ai(z) and Bi(z) [Gil et al. 2002b].

Both GIZ and HIZ call the function D1MACH to obtain the machine dependent constants (overflow and underflow numbers and the smallest relative spacing). This routine is included in the package; also, it can be retrieved from the Netlib repository (http://www.netlib.org/blas/d1mach.f).

SUBROUTINE HIZ(IFACH,X,Y,REH,IMH,REHP,IMHP,IERROH)

INPUT:
- IFACH:
  - IFACH=1, the code computes Hi(z) and Hi$'$(z).
  - IFACH=2, the code computes scaled Scorer functions in the sector $\mathrm{ph}(z) \in [-\pi/3, \pi/3]$ and unscaled Scorer functions in the rest of the complex plane.
- X: real part of the argument Z.
- Y: imaginary part of the argument Z.

OUTPUT:
- REH: real part of the Scorer function Hi(z).
- IMH: imaginary part of the Scorer function Hi(z).
- REHP: real part of the derivative of the Scorer function Hi$'$(z).
- IMHP: imaginary part of the derivative of the Scorer function Hi$'$(z).
- IERROH: error flag for overflow/underflow problems in the evaluation of unscaled Scorer functions Hi(z), Hi$'$(z). If IERROH=1, the computation was successful. If IERROH=2, the Scorer functions underflow or overflow.

The routine HIZ depends on the following subroutines (included in the code).

(1) HIZINT: implements the trapezoidal rule for Hi(z) and Hi$'$(z).
(2) HIZSER: computes the power series for Hi(z) and Hi$'$(z).
(3) HIZEXP: computes the asymptotic expansion for Hi(z) and Hi$'$(z), which is applied in the sector $2\pi/3 \le \mathrm{ph}\, z \le \pi$.
(4) Auxiliary routines:
INTT (called by HIZINT), INTU (called by INTT).

SUBROUTINE GIZ(IFACG,X,Y,REG,IMG,REGP,IMGP,IERROG)

INPUT:

IFACG:

IFACG=1, the code computes Gi(z) and Gi′(z).

IFACG=2, the code computes scaled Scorer functions in the sector $\pi/3 \leq \mathrm{ph}(z) \leq \pi$ (and the complex conjugated sector) and unscaled Scorer functions in the rest of the complex plane.

X: real part of the argument Z.

Y: imaginary part of the argument Z.

OUTPUT:

REG: real part of the Scorer function Gi(z).

IMG: imaginary part of the Scorer function Gi(z).

REGP: real part of the derivative of the Scorer function Gi′(z).

IMGP: imaginary part of the derivative of the Scorer function Gi′(z).

IERROG: error flag for overflow/underflow problems in the evaluation of unscaled Scorer functions Gi(z), Gi′(z). If IERROG = 1, the computation was successful. If IERROG = 2, the Scorer functions underflow or overflow.

The routine GIZ depends on the following subroutine (included in the code).

GIZSER: computes the power series for Gi(z) and Gi′(z).

4. COMPUTATIONAL ASPECTS

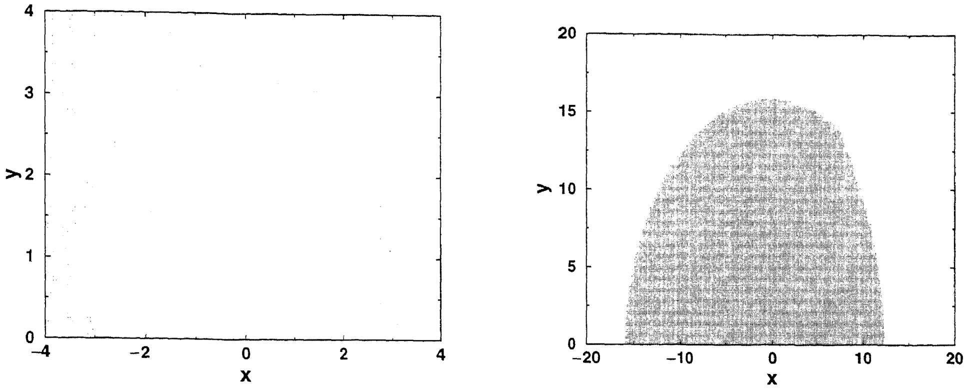
In order to determine the region of applicability of power series (Equations (10) and (12)) and asymptotic expansions (Equations (13) and (14)), we have compared these methods with integral representations. In Figure 1 we show the comparison for series (Figure 1(a)) and asymptotic expansions (Figure 1(b)). The points of discrepancy for an accuracy better than 10^{-12} for Hi(z) are plotted. As commented on in Section 2.1, the asymptotic expansion for Hi(z) is used in the sector $\mathrm{ph}(-z) \leq \pi/3$ whereas for $\mathrm{ph}(z) < 2\pi/3$ we combine Equations (4) and (13).

From the figures we conclude that, for Hi(z), a safe choice is the use of series for $|z| < 1.5$ and asymptotic expansions for $|z| > 20$. In the rest of the complex plane, integral representations and/or connection formulae are used. For Gi(z) similar arguments are considered and series are used for $|z| < 1.5$ whereas the asymptotic expansion is used for $|z| > 30$ and $|\mathrm{ph} z| < \pi/3 - 0.3$.

4.1 Numerical Verification

We are using several connection formulas in the routines, and other ones are available for checking the codes. However, these remaining formulas are trivial consequences of the ones used in the codes. Also, we could consider Wronskian relations such as, for instance [Abramowitz and Stegun 1964],

$$\mathrm{Gi}(z)\mathrm{Hi}'(z) - \mathrm{Gi}'(z)\mathrm{Hi}(z) = \frac{1}{\pi}\int_0^z \mathrm{Bi}(t)\,dt,$$



(a) (b)

Fig. 1. **(a)** Points of discrepancy for an accuracy better than 10^{-12} between series and integral representations for $\mathrm{Hi}(z)$; **(b)** Same for the discrepancy between asymptotic expansions and integral representations.

however, this relation is not suitable for checking because of the integral of $\mathrm{Bi}(z)$.

An alternative way for testing is based on local Taylor series [Cody and Stolz 1991]

$$\mathrm{Hi}(z+w) = \sum_{k=0}^{\infty} \frac{w^k}{k!} \mathrm{Hi}^{(k)}(z), \tag{17}$$

where the derivatives can be obtained from the recursion

$$\mathrm{Hi}^{(k+3)}(z) = z\mathrm{Hi}^{(k+1)}(z) + (k+1)\mathrm{Hi}^{(k)}(z) \quad k \geq 0, \tag{18}$$

which easily follows from (3). Initial values $\mathrm{Hi}(z)$ and $\mathrm{Hi}'(z)$ are computed by our code; the value of $\mathrm{Hi}^{(2)}(z)$ follows from the differential equation in (1) ($\mathrm{Hi}^{(2)}(z) = z\mathrm{Hi}(z) + (1/\pi)$). The recursion (17) also holds for derivatives of $\mathrm{Gi}(z)$.

For the scaled functions, the addition formula reads:

$$\widetilde{\mathrm{Hi}}(z+w) = e^{\zeta[1-(1+w/z)^{3/2}]} \sum_{k=0}^{\infty} \frac{w^k}{k!} \widetilde{\mathrm{Hi}}^{(k)}(z), \tag{19}$$

where $\zeta = \frac{2}{3}z^{3/2}$ and $\widetilde{\mathrm{Hi}}^{(2)}(z)$ is given now by $\widetilde{\mathrm{Hi}}^{(2)}(z) = z\widetilde{\mathrm{Hi}}(z) + (e^{-\zeta}/\pi)$; $\widetilde{\mathrm{Hi}}^{(k)}(z)$ denote scaled derivatives; that is: $\widetilde{\mathrm{Hi}}^{(k)}(z) = e^{-\zeta}\mathrm{Hi}^{(k)}(z)$.

As we next describe, this test indicates that the accuracy of the algorithms is better than 10^{-12}. The error should be interpreted as in Gil et al. [2002b] in the sense that only absolute accuracy makes sense when a function is close to a zero.

Of course, first one has to check the numerical feasibility of the accuracy test based on local Taylor series. The recurrences for the computation of the derivatives are seen to become unstable for forward computation in certain sectors of the complex plane and especially for large $|z|$; in particular, the

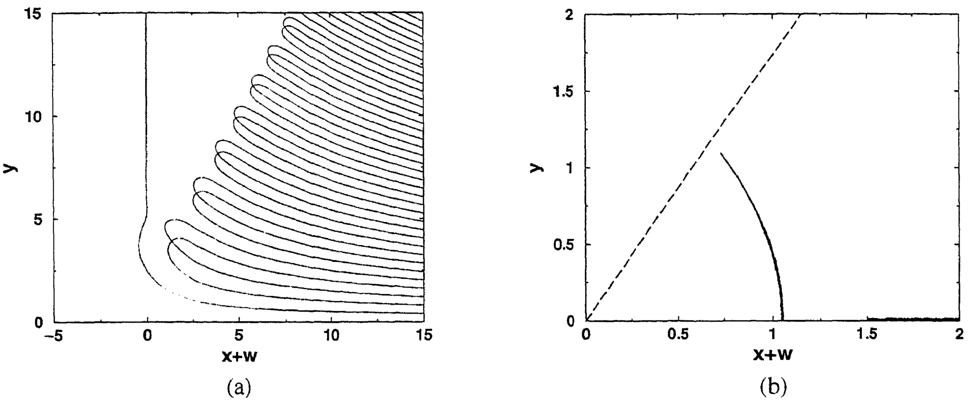
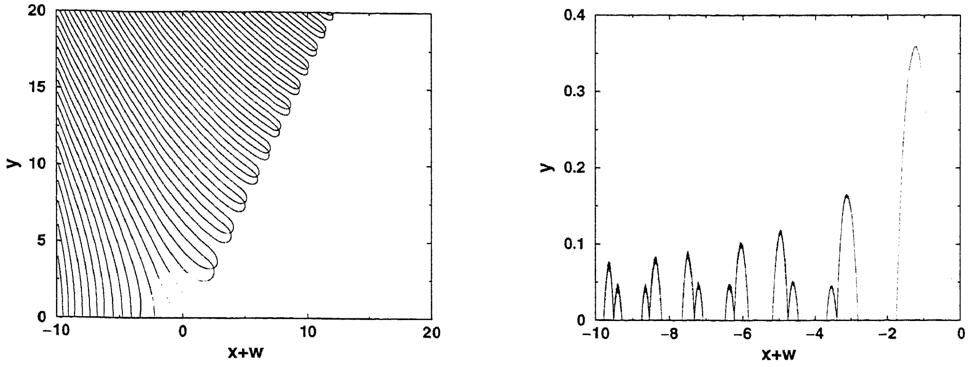


Fig. 2. Points where the relative deviations for the computation of the phase of $\mathrm{Hi}(z+w)$ (**a**) through (17) and $\widetilde{\mathrm{Hi}}(z+w)$ (**b**) through (19) are greater than 10^{-12} compared with direct computation; (b) also plots the line $\mathrm{ph}(z+w) = \pi/3$, which is the limit of validity of the scaling for $\mathrm{Hi}(z+w)$.

recurrences cannot be used to compute high derivatives of $\mathrm{Hi}(z)$ when the function is algebraically decaying as $|z| \to \infty$ (in $|\mathrm{ph}(-z)| < 2\pi/3$) and the same is true for $\mathrm{Gi}(z)$ in $|\mathrm{ph}(z)| < \pi/3$. This means that w should be chosen small enough to ensure that the number of derivatives to be calculated is small enough. We have checked that $w = 0.1$ is a reasonable selection: it is not too small (of course $w = 0$ is not a check at all), and not too large (not many derivatives are required). The number of terms needed in the Taylor series is numerically obtained by stopping the sum when the last term is negligible with respect to the accumulated sum (we force the relative contribution to be smaller than the smallest relative spacing of the machine). Precisely in the sectors where the recurrence is more unstable for large z, fewer terms of the Taylor series are needed; this is as expected given that the successive derivatives become smaller and smaller, as can be understood from their asymptotic behavior (Equations (13) and (14)). With this, the test turns out to be feasible for checking the algorithms to 10^{-12} accuracy. Indeed, we have applied Equation (17), using the recurrences with starting values $\mathrm{Hi}(z)$ and $\mathrm{Hi}'(z)$ obtained from our code and repeated the same computation with randomly perturbed initial values, with relative perturbations smaller than our accuracy claim (10^{-12}). We have checked that both computations are consistent among them within an accuracy of 10^{-12}. The same analysis has been carried out for the $\mathrm{Gi}(z)$ function.

In Figure 2 we check the errors in the evaluation of $\mathrm{Hi}(z+w)$ and $\widetilde{\mathrm{Hi}}(z+w)$ comparing the direct computation by the code HIZ and the use of Equations (17) and (19) for an accuracy of 10^{-12}. As previously noted, we take $w = 0.1$ (other selections of w give similar results provided $|w|$ is small enough).

The points of discrepancy shown in Figure 2(a) correspond to the level curves where the real or imaginary parts of $\mathrm{Hi}(z)$ vanish. The curves corresponding to $\Im\mathrm{Hi} = 0$ and $\Re\mathrm{Hi} = 0$ intersect at the complex zeros of $\mathrm{Hi}(z)$ which lie above the ray $\mathrm{ph} z = \pi/3$ [Gil et al. 2002c]. The check for the modulus shows no discrepancies for a relative accuracy of 10^{-12}, except close to the zeros of the



(a) (b)

Fig. 3. Points where the relative error in the computation of the phase of $\mathrm{Gi}(z+w)$, comparing Taylor series around $w = 0$ with the direct computation by the code GIZ, is greater than 10^{-12} (**a**). Similarly, the corresponding discrepancies found in the evaluation of the phase of $\widetilde{\mathrm{Gi}}(z+w)$ within a relative accuracy of 10^{-12} are shown (**b**).

function where only the absolute error makes sense. The vertical line reflects the fact that $\mathrm{Hi}(z)$ becomes purely imaginary as $z \to i\infty$ (Equation (13)).

Figure 2(b) corresponds to the same test for the scaled function $\widetilde{\mathrm{Hi}}(z)$ ($|\mathrm{ph} z| < \pi/3$). The arc appearing in the figure corresponds to a level curve $\Re\widetilde{\mathrm{Hi}} = 0$. No zeros of the function appear in this sector.

In Figure 3 we compute the deviations in the evaluation of $\mathrm{Gi}(z+w)$ and $\widetilde{\mathrm{Gi}}(z+w)$ comparing their direct computation with the corresponding Taylor series (17) for $\mathrm{Gi}(z+w)$ and (19) for $\widetilde{\mathrm{Gi}}(z+w)$. Points where the relative deviation is greater than 10^{-12} are plotted.

Figure 3(a) shows similar characteristics as Figure 2(a). The complex zeros of $\mathrm{Gi}(z)$ lie below the ray $\mathrm{ph} z = \pi/3$. In addition, $\mathrm{Gi}(z)$ has infinitely many negative real zeros. The same test for the modulus shows complete agreement within 10^{-12} accuracy except very close to the zeros of the function where only absolute error makes sense. Figure 3(b) shows the same check for scaled Scorer function $\widetilde{\mathrm{Gi}}(z)$ focusing in a region near the negative real axis, where the zeros of $\widetilde{\mathrm{Gi}}(z)$ (which are the real negative zeros of $\mathrm{Gi}(z)$) lie. The curves of discrepancy are the level curves $\Re\widetilde{\mathrm{Gi}} = 0$ and $\Im\widetilde{\mathrm{Gi}} = 0$, which touch at the zeros of the function. No other errors are observed for the scaled function in its sector of definition.

For the derivatives of $\mathrm{Hi}(z)$ and $\mathrm{Gi}(z)$ the results are similar, with the only addition of asymptotical level curves corresponding to zero real or imaginary parts. The function $\mathrm{Hi}'(z)$ becomes purely real on the ray $\mathrm{ph} z = \pi/2$ and purely imaginary on the ray $\mathrm{ph} z = 3\pi/4$ as $|z| \to \infty$, while, asymptotically, $\mathrm{Gi}'(z)$ becomes purely imaginary on the ray $\mathrm{ph} z = \pi/4$. See Figure 4.

All the discrepancies shown in the figures are natural and unavoidable in finite precision arithmetic. Therefore, our code is consistent with 10^{-12} accuracy, in the sense described in Gil et al. [2002b].

A further check is provided by the computation of the zeros of Scorer functions. In Gil et al. [2002c], asymptotic expansions for the real and complex zeros

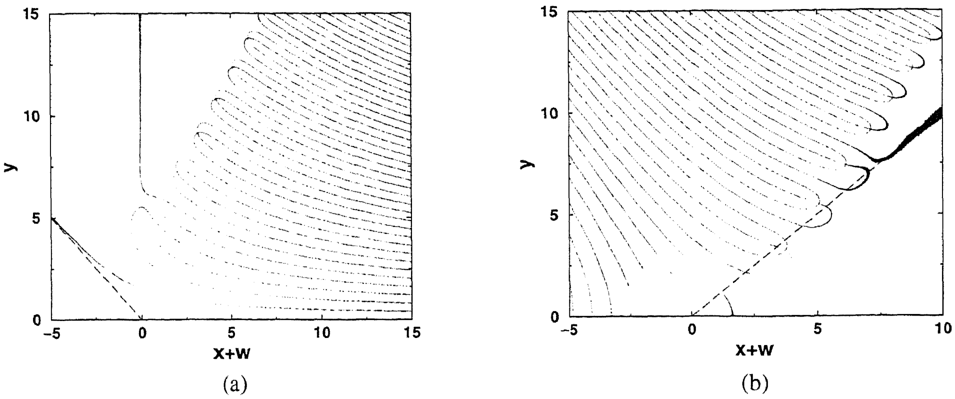


Fig. 4. Points where the relative deviations in the computation of the phase of $\mathrm{Hi}'(z+w)$ (**a**) and $\mathrm{Gi}'(z+w)$ (**b**) are greater than 10^{-12} (comparing Taylor series around $w=0$ with direct computation). The rays $\mathrm{ph}(z+w)=3\pi/4$ (**a**) and $\mathrm{ph}(z+w)=\pi/4$ (**b**) are also shown (dashed lines).

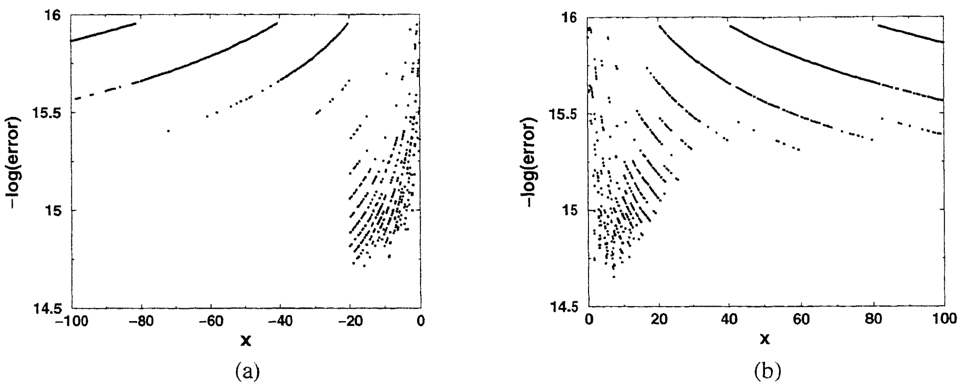


Fig. 5. $-\log_{10}(\text{error})$ for the comparison of the numerical values obtained by our code for $\mathrm{Hi}(z)$ (**a**) (interval $[-100:0]$) and $\mathrm{Gi}(z)$ (**b**) (interval $[0:100]$) with MacLeod's code.

of Scorer functions were derived. Using estimated values from the asymptotic expansions, the Newton–Raphson method, using the values of the functions and the derivatives provided by our algorithms, converged to the zeros with at least 10^{-12} accuracy.

4.2 Comparison with MacLeod's Code: Real z

As mentioned before, in MacLeod [1994] 20D coefficients of Chebyshev expansions for Gi (positive real z) and Hi (negative real z) are given. For the rest of the real axis connection formulas with Airy functions are used. We tested our code against these Chebyshev expansions.

In Figure 5(a) we plot $-\log_{10}(\epsilon)$, with ϵ the relative error when comparing the numerical values obtained by our code for $\mathrm{Hi}(z)$ with MacLeod's code. Figure 5(b) is analogous to Figure 5(a) but for $\mathrm{Gi}(z)$.

Figure 5 shows that our code is consistent with an accuracy better than 10^{-12} on the real axis. The two different regions that are apparent in the figures correspond to two different methods of computation: quadrature rules for moderate $|z|$ and asymptotic expansions for larger $|z|$. The use of series for $|z| < 1.5$ is not noticeable as a different pattern.

4.3 CPU Times

The most demanding process in the algorithm is the computation of the integral representation. Consequently, the slowest computations are for moderate values of z ($1.5 \leq |z| \leq 20$). For example, in a Pentium II 350 MHz PC (running g77 under Debian Linux 2.1), the typical CPU times for the evaluation of one value of $\mathrm{Hi}(z)$ in the principal sector ($2\pi/3 \leq |\mathrm{ph} z| \leq \pi$), are: 20 μs when series or asymptotic expansions are used and 450μs when integral representations are considered.

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