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An Algorithm for the Evaluation of the Complex Airy Functions

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The evaluation of complex Airy functions is required in the approximation of certain second-order linear differential equations arising in the treatment of multiple turning-point and energy curve-crossing problems in quantum mechanics. Pairs of numerically linearly independent solutions throughout the z-plane can be constructed from the fundamental solutions to the complex Airy equation, $Ai(z)$, $Bi(z)$, and $Ai(z\, e^{\pm 2\pi i/3})$. Integral representations for these complex functions and their derivatives are given, and being of the Stieltjes type, the integrals are evaluated using the generalized Gaussian quadrature method of Shohat and Tamarkin as implemented by Gordon. These integral representations, employed together with the Taylor series for small z and the appropriate connection formulas, allow the creation of an accurate and efficient algorithm to evaluate the complex functions over the entire z-plane. The algorithm is presented in detail at the end of this article.

1. INTRODUCTION

Recently interest in Airy functions of a complex argument has arisen in the quantum mechanical study of physical problems with complex transition points which occur in the calculation of wave functions when the energy curves have an avoided crossing

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[3, 15], in scattering problems involving complex optical potentials, and in connection with the computation of uniform asymptotic series for Weber's parabolic cylinder functions [12] which are needed in the integration of the radial Schroedinger equation for a general piecewise quadratic potential well or barrier [7, 8].

Although the solutions to the complex Airy equation have been well studied by Olver [11], no convenient algorithm for their calculation exists. Algorithms for the functions with real arguments are available, but their modification to handle complex arguments is not a straightforward task [5, 14]. The power series expansions can be used only in a small region near the origin, and the asymptotic formulas converge too slowly or not at all for moderate values of z [1]. The existing tables by Miller [9] and Woodward [17] are too limited in their range of arguments and are difficult to implement in computer calculations involved in the above-mentioned physical processes.

We present in this paper an algorithm for the evaluation of the linearly independent solutions to the complex Airy equation

$$\frac{d^2u(z)}{dz^2} - zu(z) = 0. \tag{1.1}$$

The sets $\{Ai(z), Bi(z)\}$ and $\{Ai(z\, e^{\pm 2\pi i/3})\}$, and their derivatives, are computed from Stieltjes-type integral representations. In section 2, the behavior of the functions in the complex plane is examined in order to determine the proper choice for standard solutions (i.e. a pair of numerically linearly independent solutions). In section 3, the integral representations for $Ai(z)$, $Bi(z)$, and $Ai(z\, e^{\pm 2\pi i/3})$ are developed and subsequently evaluated in section 4 using the generalized Gaussian techniques of Shohat and Tamarkin [16] as implemented by Gordon [6]. The integral representations employed together with well-known connecting formulas allow the creation of an accurate and efficient algorithm to compute the complex Airy functions over the entire z-plane which is discussed in detail in the last section.

2. Behavior of the Airy Functions in the Complex Plane

The discussion here is by no means exhaustive, but rather is intended only to set forth those properties of the Airy functions that are essential in calculating the appropriate fundamental set of solutions in the complex plane. A more complete study of their properties, particularly their asymptotic behavior, is given by Olver [11, 13].

For computations involved in physical problems with real-valued functions and functionals, such as the Wronskian, the set of linearly independent solutions normally chosen is $Ai(z)$ and $Bi(z)$. These functions are real when z is real ($z = x$) and they satisfy Miller's criteria for numerically satisfactory solutions of second-order differential equations [9]: i.e. when the coefficient of the real Airy equation is greater than zero ($x > 0$), the solutions are either exponentially decaying or growing functions as can be seen from the leading term in the asymptotic series expansion for the regular and irregular solutions

$$Ai(z) \sim \tfrac{1}{2}\pi^{-1/2}z^{-1/4}e^{-\zeta} \qquad \text{for} \quad |\arg z| < \pi \tag{2.1}$$

$$Bi(z) \sim \pi^{-1/2}z^{-1/4}e^{\zeta} \qquad \text{for} \quad |\arg z| < \pi/3 \tag{2.2}$$

where $\zeta = 2z^{3/2}/3$. In the purely oscillatory region ($x < 0$), the solutions have an asymptotic phase difference of $\pi/2$ and the same asymptotic modulus

$$Ai(-x) = \pi^{-1/2}x^{-1/4}\sin(\zeta + \pi/4) + O(x^{-7/4}) \tag{2.3}$$

$$Bi(-x) = \pi^{-1/2}x^{-1/4}\cos(\zeta + \pi/4) + O(x^{-7/4}). \tag{2.4}$$

In studying the behavior of the Airy functions for complex arguments, we can restrict the analysis to z in the upper-half plane. For conjugate values of z, the functions and their derivatives take on conjugate values:

$$\begin{aligned} Ai(z) &= Ai^*(z^*) \qquad \frac{dAi(z)}{dz} = \frac{dAi^*(z^*)}{dz^*} \\ \text{and} \qquad & \\ Bi(z) &= Bi^*(z^*) \qquad \frac{dBi(z)}{dz} = \frac{dBi^*(z^*)}{dz^*}. \end{aligned} \tag{2.5}$$

In Fig. 1 the magnitudes of $Ai(z)$ and $Bi(z)$ are plotted as functions of the polar coordinates (r, θ) locating z in the upper-half plane, and in Fig. 2 the phases of $Ai(z)$ and $Bi(z)$ for z along the semi-circle $r = 2$ are given. The phases of the complex functions differ by about ninety degrees for z in the sector $\pi/3 < \theta < \pi$ for all values of r. Upon comparing the three-dimensional plots of $Ai(z)$ and $Bi(z)$, one observes that in this region of the complex plane the functions become indistinguishable numerically,

$$\left.\begin{aligned} Ai(z) &\sim \mp iBi(z) \\ Ai'(z) &\sim \mp iBi'(z) \end{aligned}\right\} \quad (|z| \text{ large}, \ \pi/3 < |\arg z| < \pi).$$

Or to put this another way, in the computation of the Wronskian $W\{Ai(z)\}$ there is severe cancellation; indeed for sufficiently large values of $|z|$ all significant figures are lost.

In order to maintain numerically two linearly independent solutions to the differential equation in this sector, another pair of functions must be selected. In the upper-half of the z-plane, the appropriate choice is $\{Ai(z), Ai(z\, e^{-2\pi i/3})\}$. In the region $\pi/3 < \theta < \pi$, $Ai(z\, e^{-2\pi i/3})$ vanishes exponentially whereas $Ai(z)$ grows exponentially (see Figure 1) such that the Wronskian computed for this fundamental pair remains constant. In the sector $|\arg z| \leqslant \pi/3$, the function $2\, e^{-\pi i/6}\, Ai(z\, e^{-2\pi i/3})$ behaves asymptotically like $Bi(z)$. In the lower-half plane the appropriate pair of solutions

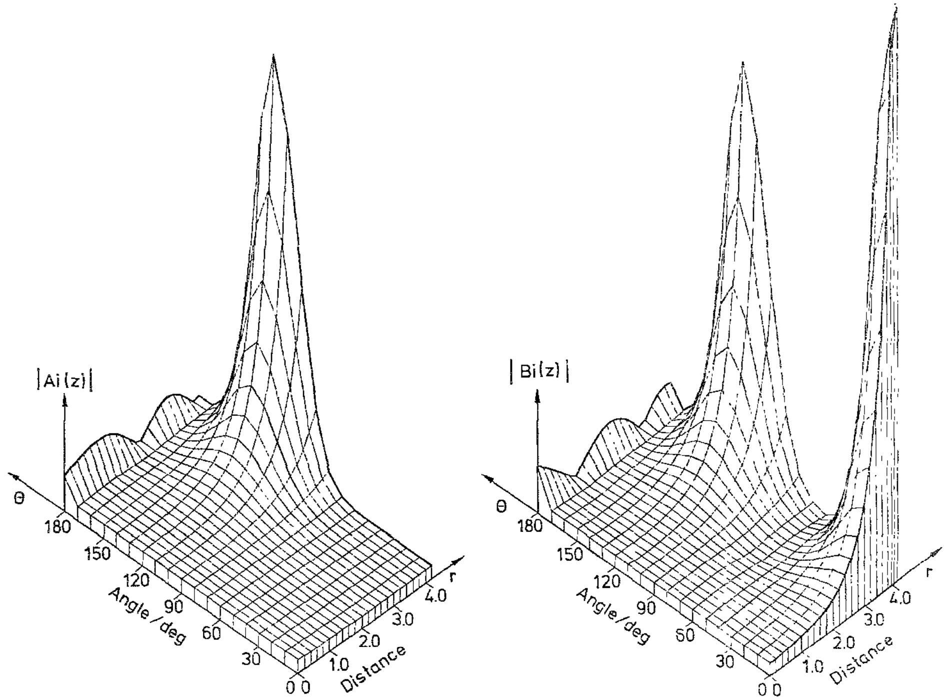

FIG. 1. Three-dimensional plots of the magnitudes of the complex Airy functions, $|Ai(z)|$ and $|Bi(z)|$, as function of the polar coordinates (r, θ) of z. (The values for $\theta = 180°$ have been enlarged to illustrate the oscillatory behavior).

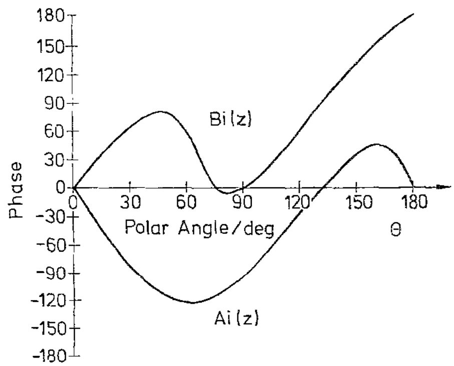

FIG. 2. Phases of the complex Airy functions $Ai(z)$ and $Bi(z)$ as a function of the polar coordinate θ, $r = 2$.

$\{Ai(z), Ai(z\, e^{+2\pi i/3})\}$. Only along the real axis and in the sector $|\arg z| < \pi/3$, does $\{Ai(z), Bi(z)\}$ constitute a pair of numerically linearly independent solutions to the complex Airy equation.

Actually, knowledge of only the solution $Ai(z)$ suffices to generate a complete table of Airy functions due to the existence of a series of useful connection formulas [1, 13]:

$$Ai(z) = e^{\pi i/3} Ai(ze^{-2\pi i/3}) + e^{-\pi i/3} Ai(ze^{2\pi i}/3) \tag{2.6}$$

$$Bi(z) = e^{\pi i/6} Ai(ze^{2\pi i/3}) + e^{-\pi i/6} Ai(ze^{-2\pi i/3}) \tag{2.7}$$

$$Bi'(z) = e^{5\pi i/6} Ai'(ze^{2\pi i/3}) + e^{-5\pi i/6} Ai'(ze^{-2\pi i/3}) \tag{2.8}$$

$$2e^{\pm\pi i/6} Ai(ze^{\pm 2\pi i/3}) = [Bi(z) \pm iAi(z)] \tag{2.9}$$

We do not need a direct algorithm for the sector $2\pi/3 < \arg z < 4\pi/3$. As long as we can compute $Ai(z)$ for $0 \leqslant \arg z \leqslant 2\pi/3$, and by conjugacy $-2\pi/3 \leqslant \arg z \leqslant 0$, the rest of the plane can be covered by the connection formulas. The evaluation of $Ai(z)$ from (2.6) in the remaining region is numerically stable, that is, no cancellation of exponentially large solutions to form an exponentially small solution occurs. Similarly, $Bi(z)$ and its derivative can be recovered in a numerically stable way from formulas (2.7) and (2.8).

3. Integral Representations for Complex Airy Functions

For z real, Gordon [5] presented integral representations for $Ai(\pm x)$ whose evaluation by a Gaussian quadrature method required only a few terms ($n = 4$). These integrals are also defined for complex z, and with the appropriate interpretation of the multivaluedness that arises in the extension to complex variables, they can be employed to compute the complex functions as well.

The integral representation for $Ai(z)$ is derived from an expression for the modified Bessel function of the second kind $K_\nu(z)$ [4a],

$$\int_0^\infty \frac{(x^{1/2})^{-1}\, e^{-x} K_\nu(x)\, dx}{x + \zeta} = \frac{\pi e^\zeta K_\nu(\zeta)}{\zeta^{1/2} \cos(\nu\pi)} \tag{3.1}$$

$$|\arg \zeta| < \pi, \qquad \mathrm{Re}(\nu) < 1/2. \tag{3.1}$$

If we set $\nu = 1/3$, $\zeta = 2z^{3/2}/3$ and substitute

$$K_{1/3}(x) = \frac{\pi\sqrt{3}}{(3x/2)^{1/3}} Ai[(3x/2)^{2/3}]$$

(3.1) can be solved for $Ai(z)$,

$$Ai(z) = \frac{1}{2}\, \pi^{-1/2} z^{-1/4} e^{-2z^{3/2}/3} \int_0^\infty \frac{\rho(x)\, dx}{1 + (3x/2z^{3/2})}$$

$$\left[|z| > 0, |\arg z| < \frac{2\pi}{3} \text{ or } |\arg \zeta| < \pi\right] \tag{3.2}$$

where

$$\rho(x) = \pi^{-1/2}2^{-11/6}3^{-2/3}x^{-2/3}e^{-x}Ai[(3x/2)^{2/3}]. \tag{3.3}$$

$\rho(x)$ is a non-negative exponentially decreasing function, and it will be shown in Section 4 that since $\rho(x)$ is a solution of a moment problem μ_k Eq. (3.2) can be asymptotically represented by the series $\sum_k \mu_k \zeta^{-k-1}$ which is identical to the usual asymptotic series in this sector [1]

$$Ai(z) \sim \tfrac{1}{2}\pi^{-1/2}z^{-1/4}e^{-\zeta}\sum^{\infty}(-)^k c_k\zeta^{-k} \quad |\arg z| < \pi.$$

There exists no integral representation for $Bi(z)$ analogous to the one for $Ai(z)$; expressions closely resembling it, however, can be derived utilizing relation (2.9) and Eq. (3.2). The resulting two expressions closely resembling it, however, can be derived utilizing relation (2.9) and Eq. (3.2). The resulting two expressions for $Bi(z)$, which are denoted Bi^+ and $Bi^-(z)$ to indicate they have different argument restrictions, are

$$Bi^+(z) = \pi^{-1/2}z^{-1/4}e^{2z^{3/2}/3}\int_0^\infty \frac{\rho(x)\,dx}{1 - 3x/2\ z^{3/2}} + iAi(z)$$
$$\left[\frac{4\pi}{3} > \arg z > 0, \text{ or } 0 < \arg\zeta < 2\pi\right] \tag{3.4}$$

$$Bi^-(z) = \pi^{-1/2}z^{-1/4}e^{2z^{3/2}/3}\int_0^\infty \frac{\rho(x)\,dx}{1 - 3x/2\ z^{3/2}} - iAi(z)$$
$$\left[-\frac{4\pi}{3} < \arg z < 0, \text{ or } -2\pi < \arg\zeta < 0\right] \tag{3.5}$$

where the *integral portions are just* $2e^{-\pi i/6}Ai(z\,e^{-2\pi i/3})$ in (3.4) *and* $2\,e^{\pi i/6}Ai(z\,e^{2\pi i/3})$ *in* (3.5). As the zeros of $Ai(z)$ are all real, these expressions can be employed to locate the zeros of $Bi(z)$.

Since the branch cut is along the positive real axis of the ζ-plane, neither $Bi^+(z)$ nor $Bi^-(z)$ is defined for z on the positive real axis. Thus one would like to examine the behaviour of these functions as $\zeta \to x_0$, where x_0 is a point far from the origin. The evaluation of the real singular integrals (i.e., the integration variable is real) which have a simple pole on the path of integration is a well-studied problem in the treatment of Cauchy integrals in complex analysis. Since $\rho(x)$ is analytic at the singularity and continuous everywhere along the path of integration except for an integrable singularity at the endpoint, we can employ the Plemelj formulas [2, 10] to determine the limiting value of the two Cauchy integrals as z approaches the real axis from above and below.

For the purposes of our discussion, let L denote the integration path. It is sufficient to require $\rho(x)$ be continuous on L and satisfy the Lipschitz condition

$$|\rho(x_1) - \rho(x_0)| < A\,|x_1 - x_0|^\mu$$

for all x_1 on L in some neighborhood of $\zeta \to x_0$, where A and μ are constants, and $0 < \mu \leqslant 1$.

The analyticity requirement on $\rho(x)$ near $\zeta = x_0$, allows us to deform the path of integration, and treat x as a complex variable. Then as $\zeta \to x_0$ from above

$$Bi^+(x) = \pi^{-1/2}x^{-1/4}e^{\zeta}\left(P\left[\int_0^\infty \frac{\rho(x')\,dx'}{1 - x'/\zeta}\right] + \int_{\Gamma_\epsilon} \frac{\rho(x')\,dx'}{1 - x'/\zeta}\right) + iAi(x) \quad (3.6)$$

and as $\zeta \to x_0$ from below

$$Bi^-(x) = \pi^{-1/2}x^{-1/4}e^{\zeta}\left(P\left[\int_0^\infty \frac{\rho(x')\,dx'}{1 - x'/\zeta}\right] + \int_{\Gamma_{\epsilon'}} \frac{\rho(x')\,dx'}{1 - x'/\zeta}\right) - iAi(x) \quad (3.7)$$

where Γ_ϵ and $\Gamma_{\epsilon'}$ are semi-circles, around the point x_0 (see Figure 3), and the principal value integral is defined

$$P\left[\int_0^\infty \frac{\rho(x')\,dx'}{1 - x'/\zeta}\right] = \lim_{\substack{\epsilon\to 0\\ R\to\infty}} \int_0^{\zeta-\epsilon} \frac{\rho(x')\,dx'}{1 - x'/\zeta} + \int_{\zeta+\epsilon}^{R} \frac{\rho(x')\,dx'}{1 - x'/\zeta} \quad (3.8)$$

FIG. 3. Integration paths for $Bi^{\pm}(x)$.

The contributions arising from semicircles Γ_ϵ, $\Gamma_{\epsilon'}$ are $\mp i\,\pi\,\rho(\zeta)$, and we can now carry out the limiting process to obtain

$$\begin{aligned} Bi^+(x) &= \pi^{-1/2}x^{-1/4}e^{\zeta}\left(P\int_0^\infty \frac{\rho(x')\,dx'}{1 - x'/\zeta} - i\pi\zeta\rho(\zeta)\right) + i\,Ai(x) \\ &= \pi^{-1/2}x^{-1/4}e^{\zeta}\left(P\int_0^\infty \frac{\rho(x')\,dx'}{1 - x'/\zeta}\right) + i\,Ai(x)(1 - 3^{-1}2^{-17/48}x^{1/4}) \end{aligned} \quad (3.9)$$

and

$$Bi^-(x) = \pi^{-1/2}x^{-1/4}e^{\zeta}\left(P\int_0^\infty \frac{\rho(x')\,dx'}{1 - x'/\zeta}\right) - i\,Ai(x)(1 - 3^{-1}2^{-17/48}x^{1/4}). \quad (3.10)$$

The addition and subtraction of (3.9) and (3.10) lead to the Plemelj formulas

$$Bi^+(x) + Bi^-(x) = 2\pi^{-1/2}x^{-1/4}e^{\zeta}\left(P\int_0^\infty \frac{\rho(x')\,dx'}{1 - x'/\zeta}\right) \quad (3.11)$$

$$Bi^+(x) - Bi^-(x) = 2i\,Ai(z) + 2\pi i\zeta\rho(\zeta)\,x^{-1/4}e^{\zeta}. \quad (3.12)$$

Since the R.H.S. of (3.12) goes exponentially to zero, $Bi(x)$ can be approximated [5] to any desired accuracy for *large* x by

$$Bi(x) \equiv 1/2[Bi^+(x) + Bi^-(x)] = \pi^{-1/2}x^{-1/4}e^{\zeta}\left(P\int_0^\infty \frac{\rho(x')\,dx'}{1 - x'/\zeta}\right). \quad (3.13)$$

A similar Cauchy integral problem must be solved in order to evaluate $Ai(z)$ by the integral equation (3.2) for z along the rays $\arg z = \pm 2\pi/3$, or equivalently $\arg \zeta = \pm\pi$. An analogous limiting process, this time with $-\zeta$, leads to the following principal value integral for $Ai(x, e^{\pm 2\pi i/3})$ when x is large:

$$2e^{\pm\pi i/6} Ai(xe^{\pm 2\pi i/3}) = \pi^{-1/2} x^{-1/4} e^{2x^{3/2}/3} \left(P \int_0^\infty \frac{\rho(x')\, dx'}{1 - 3x'/2x^{3/2}} \right). \tag{3.14}$$

As was to be expected, the R.H.S. is just the expression above for $Bi(x)$, Eq. (3.13).

4. Generalized Gaussian Quadrature Approximation

The integrals appearing in Eqs. (3.2), (3.4) and (3.5) for $Ai(z)$ and $Bi^{\pm}(z)$, respectively, can be evaluated straightforwardly by the generalized Gaussian quadrature method described below [6] [16]. With certain reservations, which will be discussed at the end of this section, the same quadrature approximation can be applied to the principal-value integrals in (3.14) and (3.13) for $Ai(x\, e^{\pm 2\pi i/3})$ and $Bi(x)$.

Initially let us consider the evaluation of $Ai(z)$, Eq. (3.2), in the region $|\arg z| < 2\pi/3$, $z \neq 0$ where the denominator has no zero. We factor the integrand into the product of two functions $\rho(x)\phi(x)$, such that $\rho(x)$ is the non-negative exponentially decreasing function in Eq. (3.3)

$$\rho(x) = \pi^{-1/2} 2^{-11/16} 3^{-2/3} x^{-2/3} e^{-x} Ai[(3x/2)^{2/3}], \tag{4.1}$$

and $\phi(x)$ is the remaining portion $1/\zeta + x$. Performing the factorization, the integral portion becomes

$$I(\zeta, \rho) = \int_0^\infty \frac{\rho(x)\, dx}{\zeta + x}. \tag{4.2}$$

Since the approximate quadrature formula corresponding to (4.2)

$$I(\zeta, \rho) \sim \sum_{i=0}^{n} \frac{w_i}{\zeta + x_i} \tag{4.3}$$

is a well-studied problem, we shall only briefly summarize the theoretical treatment of Shohat and Tamarkin [16] and the applied techniques of Gordon [6]. $\rho(x)$ is written in the argument $I(\zeta, \rho)$ to emphasize that the quadrature weights w_i and abscissae x_i are dependent on $\rho(x)$ only.

Shohat and Tamarkin's development of the quadrature approximation is based on the following observations: $\rho(x)$ is a solution to a Stieltjes moment problem whose moment μ_k can be explicitly evaluated [4b],

$$\begin{aligned} \mu_k &= \int_0^\infty x^k \rho(x)\, dx \qquad k = 0, 1, 2, \ldots \\ &= \Gamma(3k + 1/2)/54^k\, k!\, \Gamma(k + 1/2). \end{aligned} \tag{4.4}$$

Upon expanding the denominator of (4.2) in a geometric series and then integrating, we can develop an asymptotic series approximation to $I(\zeta, \rho)$, $\sum_{k=0}^{\infty} \mu_k \zeta^{-k-1}$ which is in general divergent for all ζ.

From the inverse power series one can derive a continued fraction representation $C(\zeta)$ for $I(\zeta, \rho)$

$$C(\zeta) = \cfrac{a_1}{\zeta + \cfrac{a_2}{1 + \cfrac{a_3}{\zeta + \cfrac{a_4}{1 + \cdots}}}} \tag{4.5}$$

where the a_i are determined from the μ_k. From the infinite continued fraction $C(\zeta)$, two subsequences of finite contracted fractions can be constructed: a subsequence of even approximants $A_n^e(\zeta)$ and a subsequence of odd approximants $A_n^0(\zeta)$. For each value of n either $A_n^0(\zeta)$ or $A_n^e(\zeta)$ is used to generate a set of $\{w_i, x_i\}_{i=1}^n$ such that

$$I(\zeta, \rho) \sim A_n^e(\zeta) = \sum_{i=1}^{n_e} \frac{w_i^e}{x_i^e + \zeta}$$

or

$$I(\zeta, \rho) \sim A_n^0(\zeta) = \sum_{i=1}^{n_0} \frac{w_i^0}{x_i^0 + \zeta}.$$

The algorithm to solve for the n weights and abscissae, as well as an expression for the remainder term when ζ is real and positive, has been developed by Gordon [6]. For any value of ζ, complex or real, not on $(-\infty, 0]$, the sequences $\{A_n^e\}$ and $\{A_n^0\}$ will both converge as $n \to \infty$ to $I(\rho, \zeta)$. Furthermore, when ζ is on $[0, \infty)$, $A_n^e(\zeta)$ and $A_n^0(\zeta)$ form bounds for the integral

$$A_n^e(\zeta) < I(\zeta, \rho) < A_n^0(\zeta).$$

Substituting the expression for either A_n^e or A_n^0 for $I(\zeta, \rho)$ provides a quadrature approximation to (3.2)

$$Ai(z) \sim \frac{1}{2} \pi^{-1/2} z^{-1/4} \exp(-\zeta) \sum_{i=1}^{n} \frac{w_i}{1 + x_i/\zeta} \tag{4.7}$$

Since the weights and abscissae are entirely dependent on $\rho(x)$, the same set of $\{w_i\}$ and $\{x_i\}$ can be used to approximate any integral of the form

$$\int_0^{\infty} g(x, \zeta)\, \rho(x)\, dx \sim \sum_{i=1}^{n} w_i g(x_i, \zeta)$$

in which $g(x, \zeta)$ is finite for all x and integrable with respect to $\rho(x)$.

This generalization allows us to immediately evaluate the integral in (3.4)

$$Bi^{+}(z) \sim \pi^{-1/2} z^{-1/4} e^{\zeta} \sum_{i=1}^{n} \frac{w_i}{1 - x_i/\zeta} + i\, Ai(z) \qquad [0 < \arg z < 4\pi/3]. \tag{4.8}$$

Differentiation of (3.2) and (3.4) yields integral expressions for the derivatives in which the integrands still satisfy the above criteria. Consequently this is equivalent to obtaining quadrature approximations for the derivative functions by differentiating the function approximants; for example,

$$\frac{d}{dz} Ai(z) \sim \frac{d}{dz} \frac{1}{2} \pi^{-1/2} z^{-1/4} e^{-\zeta} \sum_{i=1}^{n} \frac{w_i}{1 + x_i/\zeta}\,. \tag{4.9}$$

All the above approximants, (4.7), (4.8), and (4.9), converge to the exact functions as $n \to \infty$ whenever ζ is in the range of validity of the particular integral representation and $|\zeta| > 0$.

In practice, the principal value integral for $Ai(x\, e^{\pm 2\pi i/3})$, Eq. (3.14) is approximated for x large by the same quadrature as $Ai(z)$, Eq. (4.7); and similarly $Bi(x)$ by just the quadrature portion of Eq. (4.8). This evaluation is justified by an examination of the behavior of $\rho(x)$ and $\phi(x)$, in this case $\phi(x) = 1/(x - |\zeta|)$, $|\zeta| \gg 0$, as well as the quadrature nodes and weights.

Near the origin $\rho(x)$ goes to infinity like $x^{-2/3}$ and vanishes exponentially for large x. Consequently its main contribution to the integral occurs over a finite interval [0, 2]

$$\int_2^{\infty} \rho(x)\, dx < 2 \times 10^{-4}.$$

(Recall that the integral $\int_0^{\infty} \rho(x)\, dx$ has been normalized to 1.) Since $\rho(x)$ is positive over the range of integration and decays like $e^{-2x} x^{-5/6}$, the sign change in $\phi(x)$, as x passes from $|\zeta| - \epsilon$ to $|\zeta| + \epsilon$, has a self-cancelling effect in the evaluation of the principal value integral. Furthermore, the quadrature nodes x_i are clustered about the origin ($x_i > 0$ for all i) and the w_i give the greatest weight to the nodes lying closest to the origin. For $|\zeta|$ sufficiently greater than the largest node x_1, this distribution samples predominantly the portion of $\phi(x)$ well before the singularity. Unlike the complex integrals, no rigorous error bounds have been constructed for the approximate quadrature to the principal value integrals. In general, as the number of terms N in the quadrature approximation is increased, we must go to larger $|\zeta|$ before applying the quadrature formulas.

5. Algorithm and Discussion

The conjugacy property of the Airy function Eq. (2.5) allows us to limit the discussion of their evaluation to z in the upper-half plane. Using the connection formulas in Section 2, the approximate quadratures in Section 4, and the Taylor expansions

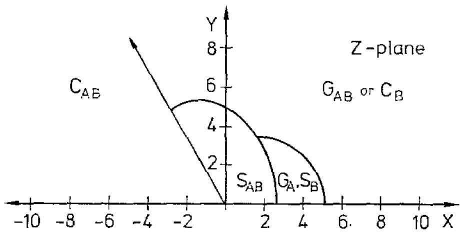

FIG. 4. Computing regions for evaluating Airy functions to Single Precision (UNIVAC 1108).

given below, single and double precision algorithms to calculate the Airy functions $Ai(z)$, $Bi(z)$, and $Ai(z\, e^{\pm 2\pi i/3})$ and their derivatives for complex values of z can be developed. Single precision, meaning 6–7 significant digits, values of the functions $Ai(z)$ and $Bi(z)$ have been computed on an Univac 1108 system employing the two computational methods as depicted in Fig. 4. In the bounded regions about the origin, the label S denotes use of the power series [1]

$$\begin{aligned} Ai(z) &= c_1 f(z) - c_2 g(z) \\ Bi(z) &= \sqrt{3}\,[c_1 f(z) + c_2 g(z)] \end{aligned} \tag{5.1}$$

where $c_1 = Ai(0) = 3^{-2/3}/\Gamma(2/3)$ and $c_2 = -Ai'(0) = 3^{-1/3}/\Gamma(1/3)$, and

$$f(z) = \sum_0^\infty 3^k \left(\frac{1}{3}\right)_k \frac{z^{3k}}{(3k)!}$$

$$g(z) = \sum_0^\infty 3^k \left(\frac{2}{3}\right)_k \frac{z^{3k+1}}{(3k+1)!}$$

with Pochhammer's symbol $(a)_k = \Gamma(a+k)/\Gamma(a)$. The G denotes *direct* use of the generalized Gaussian quadrature formulas, Eqs. (4.7) and (4.8), for the correct angle restriction, and C evaluation by the connection formulas (2.6) and (2.7). G_A on the ray $\arg z = 2\pi/3$ and G_B on the real positive axis refer to the Gaussian quadrature of the principal value integrals (3.14) and (3.13). The partial ellipse, within which only the power series are used, has its center at $(-0.65, 0.92)$. The major and minor axes are 4.5 and 3.2, and the orientation angle is 17°. For z in those regions marked G_A or G_B, the functions are computed by the quadrature formulae with a *maximum of four terms.* The nodes x_i, weights w_i, and number of terms as a function of the magnitude of z for the single precision version are given in Tables I–IV. The center and radius of the area (G_A, S_B) are (1.65,–0.05) and 3.4.

The elliptical boundary was chosen in order to satisfy the various restrictions imposed by the computational methods, particularly along the rays $\arg z = 0$ and $2\pi/3$. For example, although the series (5.1) have an infinite radius of convergence, the series for $Ai(z)$ becomes numerically unstable in the sector $|\arg z| < \pi/3$ outside the region S_{AB}. In that sector, $Ai(z)$ goes asymptotically to zero, and inaccuracies

TABLE I

Number of Terms in Quadrature Formulas to Compute Airy Functions to Single Precision (UNIVAC 1108)

z	$\arg z$	$Ai(z)$	$Bi(z)$
$\lvert z \rvert \geqslant 11$	$\leqslant \frac{2\pi}{3}$	2 term	2 term
$5 < \lvert z \rvert < 11$[a]	$\leqslant \frac{2\pi}{3}$	4 term	4 term
$2.5 < \lvert z \rvert < 5$[a]	$\leqslant \frac{\pi}{3}$	4 term	power series

[a] These are approximate values. For the precise boundary see Fig. 4.

TABLE II

4-term Generalized Gaussian Integration for Airy Functions

i	x_i	w_i
1.	3.9198329554455091	4.7763903057577263(−05)
2.	1.6915619004823504	4.9914306432910959(−03)
3.	5.0275532467263018(−01)	8.6169846993840312(−02)
4.	1.9247060562015692(−02)	9.0879095845981102(−01)

TABLE III

2-term Generalized Gaussian Integration for Airy Functions

i	x_i	w_i
1.	1.0592469382112378	3.1927194042263958(−02)
2.	3.6800601866153044(−02)	9.6807280595773604(−01)

TABLE IV

1-term Generalized Gaussian Integration for Airy Functions

i	x_i	w_i
1.	0.069444444........	1.0

arise due to the round-off errors. Growth of the round-off errors is reduced by evaluating the series term by term, $Ai(z) = \sum_{n=1}^{M} [c_1 f_n(z) - c_2 g_n(z)]$, where $f_n(z)$ and $g_n(z)$ are the nth terms in the expressions for $f(z)$ and $g(z)$. Prince [14] has shown for *negative real* values of z that the convergence can be extended further by rearranging the power series in Chebyshev polynomial expansions. In principle this technique could be applied for complex values of z to provide a smoother transition to the quadrature formulae.

Along the ray $\arg z = 2\pi/3$, the integral representation for $Ai(z)$, or rather the principal value integral for $Ai(x\, e^{-2\pi i/3})$, is still evaluated by the quadrature (4.7). The quadrature approximation has a singularity at each node x_i ; and therefore, as we discussed in Section 4, we can only use it when $|\zeta| = |2z^{3/2}/3|$ is greater than the largest node. For $n = 4$, we see from Table II that this restriction implies $|\zeta| > x_1 = 3.9$, for z on or near the ray $\arg z = 2\pi/3$. Since $Ai(z)$ is an exponentially increasing function in the region $\pi/2 < \arg z \leqslant 2\pi/3$, we can accurately extend the use of its power series.

One notes that the domains S_{AB} and S_B do not completely overlap. For z in the portion of S_B near the real axis, we are faced with a problem analogous to the one above for $Ai(z)$: ζ lies too close to the quadrature nodes to accurately use the quadrature approximation (4.8) for $Bi^+(z)$ and its principal value integral.

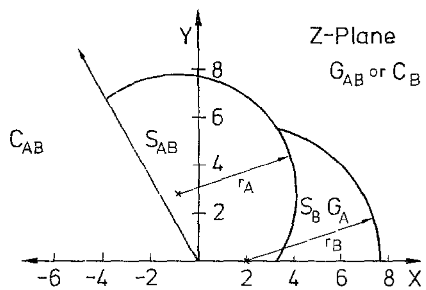

FIG. 5. Computing regions for evaluating Airy functions to Double Precision (IBM 360).

More precise values, 11–14 significant digits, of the Airy functions can be obtained using complex double precision arithmetic on an IBM 360. The computing domains are shown in Fig. 5. The circle S_{AB} is centered at $(-0.90, 2.80)$ with a radius $r_{AB} = 4.97$, and the circle S_B is centered at $(2.0, 0.0)$ with a radius $r_B = 5.53$. The nodes, weights, and number of terms in the quadrature formulae are given in Tables V and VI. A maximum of 6 terms is now needed to generate the more precise values. The lower range of accuracy, 6 in the single precision and 11 in the double precision version, exists only along the boundaries of S_{AB} and S_B. The transition to higher accuracy is achieved within a band-width less than 2.0.

As we have discussed in Section 2, the pair of linearly independent solutions $\{Ai(z), Bi(z)\}$ become indistinguishable numerically for large $|z|$ in the sector $\pi/3 < \arg z < \pi$, and the more appropriate pairs of solutions are $\{Ai(z), Ai(z\, e^{-2\pi i/3})\}$ for z in the

TABLE V

Number of Terms in Quadrature Formulas to Compute Airy Functions to Double Precision (IBM 360)

z	$\arg z$	$Ai(z)$	$Bi(z)$
$\|z\| > 15$	$\leqslant \frac{2\pi}{3}$	4 term	4 term
$7 < \|z\| \leqslant 15$[a]	$\leqslant \frac{2\pi}{3}$	6 term	6 term
$3.3 < \|z\| < 7$[a]	$\leqslant \frac{\pi}{3}$	6 term	power series

[a] These are approximate values. For the precise boundary see Fig. 5.

TABLE VI

6-term Generalized Gaussian Integration for Airy Functions

	x_i	w_i
1.	7.1620871339075440	4.9954496303045166(−08)
2.	4.2311006706187214	1.8066384626280827(−05)
3.	2.3361772245064852	9.5530673977919037(−04)
4.	1.0856431202004936	1.5715675321710695(−02)
5.	3.3391648924379639(−01)	1.1588902608004444(−01)
6.	1.3115888501576988(−02)	8.6742187551934309(−01)

upper-half plane and $\{Ai(z), Ai(z\, e^{2\pi i/3})\}$ in the lower-half plane. Using the conjugacy property (2.5), $Ai(z\, e^{\pm 2\pi i/3})$ can be evaluated *directly* from the algorithm for $Ai(z)$ described above. The single precision algorithm for the pair $\{Ai(z), Ai(z\, e^{-2\pi i/3})\}$ is summarized in Fig. 6 where the label A_- denotes $Ai\,(z\, e^{-2\pi i/3})$.

The function values have been tested against existing tables [9, 17], the double precision power series where reasonable, and the standard asymptotic expansions [1]. In Table VII values computed from the single-precision quadrature (or connection) formulas for z along the semicircle $r = 6$ are compared to the double precision power series values. The order of magnitude of the relative error (the maximum of the relative errors in the real and imaginary parts) is written in brackets beside the single precision values. As a further check on the algorithm the Wronskian $W[Ai(z), Ai(z\, e^{-2\pi i/3})] = \frac{1}{2}\pi^{-1}e^{\pi i/6}$, was computed throughout the complex plane. Deviations from its constant value indicate rapidly an error or inappropriate selection of a pair of solutions.

TABLE VII

Comparision of Single-Precision Quadrature to Double-Precision Power Series Evaluation for $|z| = 6$

arg z	$Ai(z)^a$		$Bi(z)^a$		$Ai(z\, e^{-2\pm i/3})^b$	
0	.99476941 − 05	.00000000(0)	.65364460 + 04	.00000000(−8)	.28303641 + 04	.1634115 + 04(−8)
	.99476941 − 05[c]	.00000000	.65364461 + 04	.00000000	.28303642 + 04	.1634115 + 04
30	.12599595 − 03	−.12247815 − 03(0)	.32294434 + 03	.18009920 + 03(0)	.94814177 + 02	.15872124 + 03(−8)
	.12599595 − 03	−.12247815 − 03	.32294434 + 03	.18009920 + 03	.94814180 + 02	.15872124 + 03
60	−.14580855 + 00	.10584944 + 00(−8)	−.46424671 + 00	−.18333662 + 00(−8)	−.14580855 + 00	−.10584944 + 00(−8)
	−.14580855 + 00	.10584945 + 00	−.46424672 + 00	−.18333662 + 00	−.14580855 + 00	−.10584945 + 00
90	.94814177 + 02	−.15872124 + 03(−8)	.15872157 + 03	.94814262 + 02(−8)	.12599595 − 03	.12247815 − 03(0)
	.94814180 + 02	−.15872124 + 03	.15872158 + 03	.94814266 + 02	.12599595 − 03	.12247815 − 03
120	.28303641 + 04	−.16341115 + 04(−8)	.16341115 + 04	.28303641 + 04(−8)	.99476941 − 05	.00000000(0)
	.28303642 + 04	−.16341115 + 04	.16341115 + 04	.28303642 + 04	.99476941 − 05[c]	.00000000
150	.18486388 + 03	−.27508200 + 01(−7)	.27509148 + 01	.18486354 + 03(−6)	.12599595 − 03	−.12247815 − 03(0)
	.18486388 + 03	−.27508211 + 01	.27509169 + 01	.18486355 + 03	.12599595 − 03	−.12247815 − 03
180	−.32914517 + 00	.00000000(0)	−.14669837 + 00	.00000000(−8)	−.14580855 + 00	.10584944 + 00(−8)
	−.32914517 + 00	.00000000	−.14669838 + 00	−.00000000	−.14580855 + 00	.10584945 + 00

[a] For arg $z > 120$, values obtained by combined use of quadrature and connection formulas.
[b] Values obtained from direct use of quadrature formula for $Ai(z)$.
[c] Value from local Taylor expansion.

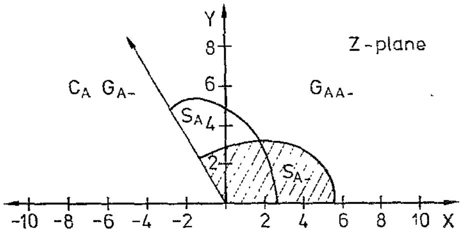

FIG. 6. Single Precision algorithm for $\{Ai(z), Ai(ze^{-2\pi i/3})\}$.

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