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Asymptotics and zero distribution of Padé polynomials associated with the exponential function

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Abstract

The polynomials P_n and Q_m having degrees n and m , respectively, with P_n monic, that solve the approximation problem

$$P_n(z)e^{-z} + Q_m(z) = \mathcal{O}(z^{n+m+1})$$

will be investigated for their asymptotic behavior, in particular in connection with the distribution of their zeros. The symbol \mathcal{O} means that the left-hand side should vanish at the origin at least to the order $n + m + 1$. This problem is discussed in great detail in a series of papers by Saff and Varga. In the present paper, we show how their results can be obtained by using uniform expansions of integrals in which Airy functions are the main approximants. We give approximations of the zeros of P_n and Q_m in terms of zeros of certain Airy functions, as well of those of the remainder defined by $E_{n,m}(z) = P_n(z)e^{-z} + Q_m(z)$. © 1997 Elsevier Science B.V. All rights reserved.

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1. Introduction

It is well known (cf. [9]) that the solution of the Padé approximation problem for the exponential function, namely,

$$P_n(z)e^{-z} + Q_m(z) = \mathcal{O}(z^{n+m+1}) \quad \text{as } z \rightarrow 0,$$

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where P_n and Q_m are polynomials of degree n and m , respectively, with P_n monic, is given by

$$P_n(z) = \frac{1}{m!} \int_0^\infty t^m (t+z)^n e^{-t} dt,$$

$$Q_m(z) = \frac{-1}{m!} \int_0^\infty t^n (t-z)^m e^{-t} dt.$$

Explicit forms are (cf. [9, p. 433])

$$P_n(z) = n! \sum_{k=0}^n \binom{m+n-k}{m} \frac{z^k}{k!},$$

$$Q_m(z) = -n! \sum_{k=0}^m \binom{m+n-k}{n} \frac{(-z)^k}{k!}.$$

Let the remainder $E_{n,m}$ be defined by

$$E_{n,m}(z) = P_n(z) e^{-z} + Q_m(z)$$

then

$$E_{n,m}(z) = \frac{(-1)^m z^{m+n+1}}{m!} \int_0^1 u^n (1-u)^m e^{-uz} du.$$

The quantities $P_n, Q_m, E_{n,m}$ can be expressed in terms of (confluent) hypergeometric functions and Laguerre polynomials. We have

$$P_n(z) = U(-n, -n-m, z)$$

$$= z^{n+m+1} U(m+1, n+m+2, z)$$

$$= (-1)^n n! L_n^{-n-m-1}(z),$$

$$Q_m(z) = -\frac{n!}{m!} U(-m, -n-m, -z)$$

$$= -\frac{n!}{m!} (-z)^{n+m+1} U(n+1, n+m+2, -z)$$

$$= -(-1)^m n! L_m^{-n-m-1}(-z),$$

$$E_{n,m}(z) = \frac{(-1)^{m+1} n! z^{n+m+1}}{(n+m+1)!} M(n+1, n+m+2, -z)$$

$$= \frac{(-1)^{m+1} n! z^{n+m+1}}{(n+m+1)!} e^{-z} M(m+1, n+m+2, z).$$

For the diagonal case $n=m$ these functions can be written in terms of Bessel functions.

We have the following symmetry. Write

$$P_n(z) = P(n, m, z), \quad Q_m(z) = Q(n, m, z).$$

Then

$$m!P(n, m, z) = -n!Q(m, n, -z).$$

For investigating the asymptotic behavior of the functions it is convenient to use the following contour integrals:

$$P_n(z) = \frac{(-1)^n n!}{2\pi i} \int_{\mathcal{C}_0} \frac{e^{-zw}}{w^{n+1}(w+1)^{m+1}} dw, \tag{1.1}$$

$$Q_m(z) = \frac{(-1)^n n! e^{-z}}{2\pi i} \int_{\mathcal{C}_{-1}} \frac{e^{-zw}}{w^{n+1}(w+1)^{m+1}} dw, \tag{1.2}$$

where $\mathcal{C}_0, \mathcal{C}_{-1}$ are small circles around the points 0 and -1 . It follows that

$$E_{n,m}(z) = \frac{(-1)^n n! e^{-z}}{2\pi i} \int_{\mathcal{C}} \frac{e^{-zw}}{w^{n+1}(w+1)^{m+1}} dw, \tag{1.3}$$

where \mathcal{C} is a circle around the points 0 and -1 .

In a sequence of papers, Saff and Varga investigated the polynomials P_n, Q_m and the remainder $E_{n,m}$, and the distribution of their zeros, for large values of n, m with fixed ratio $\sigma = m/n$ (the final paper appeared in 1978). They used saddle point methods for the integrals defining the U - and M -functions (not the contour integrals) and found curves in the complex z -plane along which the zeros are cumulating. For $m=0$ their results agree with the earlier results obtained by Szegő on the distribution of the zeros of the exponential polynomial

$$e_n(z) = \sum_{k=0}^n \frac{z^k}{k!}.$$

The purpose of the paper is:

- To give a new approach for locating the zeros of the quantities P_n, Q_m and $E_{n,m}$ by using uniform asymptotic approximations for these functions in terms of Airy functions.
- To give approximate values of the zeros of P_n, Q_m and $E_{n,m}$ in terms of zeros of certain Airy functions.
- To become familiar with methods that possibly can be used in the more complicated quadratic Hermite–Padé Type I approximation problem for the exponential function, which problem is discussed in [4].

In Section 2, we consider the diagonal case $n = m$. In [5] this has been done by using the Sommerfeld integrals for the corresponding Bessel functions. Now we use different integrals in order to become familiar with the more difficult general case, which we consider in Section 3. In that section we also give approximations of the zeros of P_n, Q_m and $E_{n,m}$ in terms of zeros of Airy functions. In addition, we compare our description of the curves along which the zeros accumulate with that of [11]. In Section 4 we give more details on uniform Airy-type expansions, and how to obtain asymptotic expansions for the zeros of functions approximated in this way, with applications to $P_n, Q_m, E_{n,m}$. In Section 5 we give more details on the conformal mapping used in Section 3, and in Section 6 we discuss aspects of numerical calculations based on the expansions for the zeros of $P_n, Q_m, E_{n,m}$. We give an interpretation of the zeros of P_n, Q_m in the lower half-plane, and in connection with this we discuss the singularities of a parameter η occurring in the expansions. In Section 7 we give a few remarks on the quadratic Hermite–Padé Type I approximations to the exponential function.

2. The diagonal case ($n = m$)

In [5] we have shown for the case $n = m$ how we can use relations between P_n, Q_n and $E_{n,n}$ and Bessel functions to obtain Airy-type approximations. In the present section we show how the same results can be obtained by using the integrals given in (1.1)–(1.3). These integrals are more difficult to handle than the integrals used in our earlier paper for the Bessel functions; there we used the Sommerfeld integrals. We start with the diagonal case, because it gives a good introduction to the general case.

We consider (1.1) and write the integral in the form

$$P_n(2izn) = \frac{(-1)^n n!}{2\pi i} \int_{\mathcal{C}_0} \frac{e^{-n\phi(w)}}{w(w+1)} dw, \quad (2.1)$$

where the phase function ϕ is given by

$$\phi(w) = 2izw + \ln w + \ln(w+1),$$

and \mathcal{C}_0 is a contour around the origin. Because of the logarithms the function ϕ is not single valued on a circle around the origin. However, in the asymptotic analysis we deform the original contour and extend it to infinity (in such a way that $\Im izw = 0, \Re izw > 0$ along the path at infinity). We introduce branch lines for $\ln w$ and $\ln(w+1)$, starting from $w = 0, w = -1$, respectively, into that direction. For example, when $z = 1 + i$, we have $izw = -u - v + i(u - v)$, where we write $w = u + iv$. Hence, the branch line for $\ln w$ runs from the origin along the diagonal $u = v$ with $u \leq 0, v \leq 0$. Furthermore, in this example we assume that the phase of w belongs to the interval $[-\frac{3}{4}\pi, \frac{5}{4}\pi]$.

The saddle points are

$$w^\pm = -\frac{1}{2} + \frac{1}{2z}(1 \pm \sqrt{1 - z^2}) = -\frac{1}{2} + \frac{1}{2}ie^{\pm i\tau}, \quad z = \frac{1}{\cosh \tau}. \quad (2.2)$$

We take $0 < z \leq 1, \tau \geq 0$; later we take z complex, in particular in a neighborhood of $z = 1$. We see that the saddle points are located on the vertical line $\Re w = -\frac{1}{2}$. Writing $w = -\frac{1}{2} + \frac{1}{2}iv$, we obtain

$$\phi(-\frac{1}{2} + \frac{1}{2}iv) = -z\tau + \ln(1 + v^2) - \ln 4 + i(\pi - z).$$

Hence, $\Im \phi(w)$ is constant on the vertical line $\Re w = -\frac{1}{2}$, on which two saddle points are located. Consequently, we expect that a saddle point contour, defined by $\Im \phi(w) = \Im \phi(w^\pm)$ runs through both saddles w^+ and w^- .

In Fig. 1 we give the contours of steepest descent and steepest ascent. The contour for P_n starts at $-i\infty$ over the path indicated by ABC . The path for Q_n runs along CBD , and the path for $E_{n,n}$ along ABD . The integrals for P_n and Q_n pick up their main contribution at the saddle point w^- , whereas the integral for $E_{n,n}$ obtains its main contribution at w^+ . From w^- two paths of ascent are running to the poles at $w = -1, w = 0$. The path from w^+ to $+i\infty$ through E is also a path of ascent. The picture is made for the case $z = 0.9$.

In Fig. 2 we give the location of saddle points and the paths of steepest descent for the case $z = 1.75$. The saddle point contours are: AB^-C^- for P_n , C^+B^+D for Q_n , $AB^-C^- \cup C^+B^+D$ for $E_{n,n}$. From w^\pm two ascent paths run to the poles at $w = -1, w = 0$, from w^\pm two ascent paths run through E^\pm to $i\infty$.

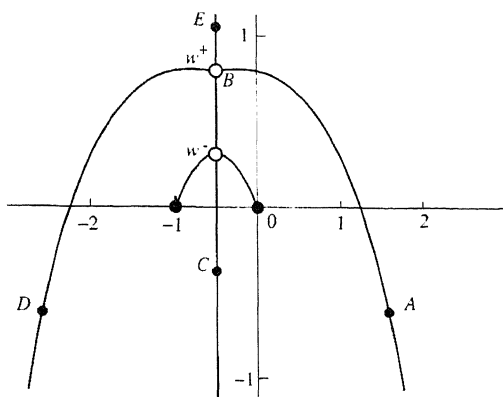


Fig. 1. The saddle point contours of the integral in (2.1) through the saddles at w^\pm for the case $z = 0.9$: ABC for P_n , CBD for Q_n , and ABD for $E_{n,n}$.

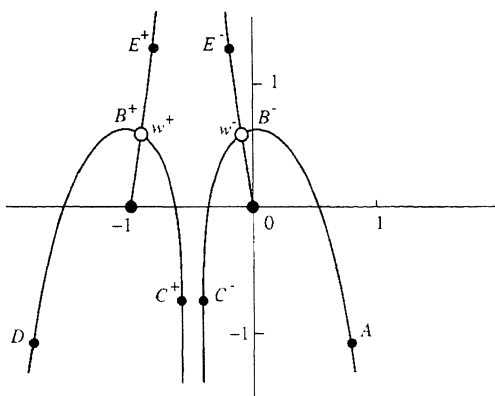


Fig. 2. The saddle point contours of (2.1) through the saddles at w^\pm for the case $z = 1.75$. Saddle point contours are: AB^-C^- for P_n , C^+B^+D for Q_n , $AB^-C^- \cup C^+B^+D$ for $E_{n,n}$.

We transform the integral into an Airy-type integral by using the cubic transformation

$$\phi(w) = -\frac{1}{3}\zeta^3 + \eta\zeta + A, \tag{2.3}$$

where A and η do not depend on w and are determined by the condition that the saddle point w^\pm in the w -plane should correspond to the saddle points $\pm\sqrt{\eta}$ in the ζ -plane, i.e.

$$\phi(w^+) = \frac{2}{3}\eta^{3/2} + A, \quad \phi(w^-) = -\frac{2}{3}\eta^{3/2} + A. \tag{2.4}$$

This gives, using (2.2),

$$A = -iz - 1 + \pi i - \ln(2z), \tag{2.5}$$

$$\frac{2}{3}\eta^{3/2} = \tau - \tanh \tau = \operatorname{arctanh} \sqrt{1 - z^2} - \sqrt{1 - z^2}.$$

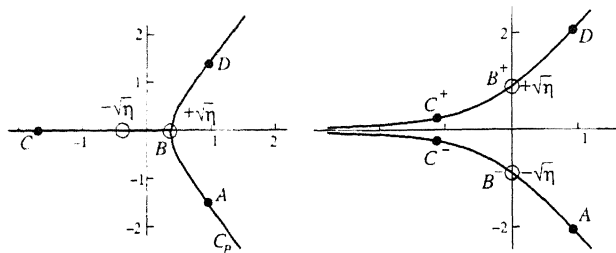


Fig. 3. The contours in the ζ -plane and points A, B, C, D that correspond to the points on the contours on the w -plane of Figs. 1 (with $z = 0.9$) and 2 (with $z = 1.75$), with saddle points (open circles) at $\pm\sqrt{\eta}$.

The contour in the w -plane is transformed into a contour, say \mathcal{C}_p , in the ζ -plane. In Fig. 3 we show corresponding points of paths in both planes of the mapping defined in (2.3) for $z = 0.9$ and $z = 1.75$. The path \mathcal{C}_p used in (2.6) is the path through A, B, C .

Integrating in the opposite direction on \mathcal{C}_p , which introduces a minus sign, we obtain

$$P_n(2izn) = -(-1)^n n! e^{-nz} \frac{1}{2\pi i} \int_{\mathcal{C}_p} e^{\frac{1}{3}\zeta^3 - \eta\zeta} g(\zeta) d\zeta, \tag{2.6}$$

where

$$g(\zeta) = \frac{1}{w(w+1)} \frac{dw}{d\zeta}. \tag{2.7}$$

We also have, by using (2.4),

$$\frac{dw}{d\zeta} = \frac{(\eta - \zeta^2)w(w+1)}{2izw(w+1) + 2w+1} \tag{2.8}$$

and

$$g(\zeta) = \frac{\eta - \zeta^2}{2izw(w+1) + 2w+1}. \tag{2.9}$$

A first approximation in terms of an Airy function follows by replacing $g(\zeta)$ with $g_0 = \frac{1}{2}[g(\sqrt{\eta}) + g(-\sqrt{\eta})]$. We give the result for the three quantities together:

$$\begin{aligned} P_n(2izn) &\sim -n! e^{n+inz} (2z)^n n^{-1/3} g_0 e^{-2\pi i/3} \text{Ai}(\eta n^{2/3} e^{-2\pi i/3}), \\ Q_n(2izn) &\sim -n! e^{n-inz} (2z)^n n^{-1/3} g_0 e^{+2\pi i/3} \text{Ai}(\eta n^{2/3} e^{+2\pi i/3}), \\ E_{n,n}(2izn) &\sim +n! e^{n-inz} (2z)^n n^{-1/3} g_0 \text{Ai}(\eta n^{2/3}). \end{aligned} \tag{2.10}$$

In order to evaluate g_0 , we need in (2.7) $dw/d\zeta$, evaluated at $\zeta = \pm\sqrt{\eta}$. By using l'Hôpital's rule in (2.8) we have

$$\left(\frac{dw}{d\zeta}\right)^2 \Big|_{\zeta=\sqrt{\eta}} = \frac{\sqrt{\eta}w^+(w^+ + 1)}{\tanh \tau},$$

$$\begin{aligned} g(\sqrt{\eta}) &= \frac{\eta^{1/4}}{\sqrt{\tanh \tau}} \frac{1}{\sqrt{w^+(w^+ + 1)}} \\ &= \frac{-2i\eta^{1/4}}{\sqrt{\tanh \tau(1 + e^{2\tau})}} \\ &= -i\sqrt{z}e^{-\frac{1}{2}\tau} \left(\frac{4\eta}{1 - z^2}\right)^{1/4}, \end{aligned}$$

and

$$\left(\frac{dw}{d\zeta}\right)^2 \Big|_{\zeta=-\sqrt{\eta}} = \frac{\sqrt{\eta}w^-(w^- + 1)}{\tanh \tau},$$

$$\begin{aligned} g(\sqrt{-\eta}) &= \frac{\eta^{1/4}}{\sqrt{\tanh \tau}} \frac{1}{\sqrt{w^-(w^- + 1)}} \\ &= \frac{-2i\eta^{1/4}}{\sqrt{\tanh \tau(1 + e^{-2\tau})}} \\ &= -i\sqrt{z}e^{+\frac{1}{2}\tau} \left(\frac{4\eta}{1 - z^2}\right)^{1/4}. \end{aligned}$$

This gives

$$g_0 = -i\sqrt{z} \cosh \frac{1}{2}\tau \left(\frac{4\eta}{1 - z^2}\right)^{1/4}. \tag{2.11}$$

We have mentioned that, when $n = m$, we may also use Sommerfeld-type integrals to do the asymptotic analysis of P_n, Q_n and $E_{n,n}$. This arises from the fact that P_n, Q_n and $E_{n,n}$ can be expressed in terms of Hankel and Bessel functions (cf. [5]). The asymptotic approximations obtained via the Sommerfeld integral representations are the same as those in (2.10).

3. The general case

We write (1.1) in the form

$$P_n[z(n + m)] = \frac{(-1)^n n!}{2\pi i} \int_{\sigma_0} e^{-n\phi(w)} \frac{dw}{w(w + 1)}, \tag{3.1}$$

where

$$\phi(w) = (1 + \sigma)zw + \ln w + \sigma \ln(w + 1), \quad \sigma = \frac{m}{n}, \tag{3.2}$$

and \mathcal{C}_0 is a contour around the branch cut of $\ln w$, that starts at $w = 0$ and terminates at ∞ in the valley of $\exp(-zw)$. The saddle points are

$$w^\pm = \frac{-z - 1 \mp g_\sigma(z)}{2z}, \quad g_\sigma(z) = \sqrt{(z - e^{i\theta})(z - e^{-i\theta})}, \tag{3.3}$$

where $\theta \in (0, \pi)$ is the number that is defined by $\sigma = \tan^2 \frac{1}{2}\theta$.

We concentrate on values of z with $\Im z > 0$, in particular on values near the point $\exp(i\theta)$; when z assumes this value, the two saddle points w^\pm coincide. The cubic transformation

$$\phi(w) = -\frac{1}{3}\zeta^3 + \eta\zeta + A, \tag{3.4}$$

with corresponding points $w = w^\pm \Leftrightarrow \zeta = \pm\sqrt{\eta}$, gives

$$P_n[z(n+m)] = \frac{(-1)^n n! e^{-nA}}{2\pi i} \int_{\mathcal{C}_p} e^{n(\frac{1}{3}\zeta^3 - \eta\zeta)} f(\zeta) d\zeta, \tag{3.5}$$

where

$$f(\zeta) = \frac{1}{w(w+1)} \frac{dw}{d\zeta} = \frac{\eta - \zeta^2}{(1 + \sigma)zw(w+1) + w + 1 + \sigma w},$$

$$\frac{4}{3}\eta^3 = \phi(w^+) - \phi(w^-)$$

$$= (1 + \sigma)z(w^+ - w^-) + \ln \frac{w^+}{w^-} + \sigma \ln \frac{w^+ + 1}{w^- + 1},$$

$$2A = \phi(w^+) + \phi(w^-),$$

and \mathcal{C}_p is the image in the ζ -plane of the path C_0 in the w -plane under the map defined in (3.4). When $z \in (0, 1)$, \mathcal{C}_p has the form as in Fig. 3.

As will be explained in Section 5 we need information on the domain of holomorphy of $f(\zeta)$ in order to be able to construct a uniform Airy-type expansion for $P_n[z(n+m)]$ when n is large, in particular for values of z (or η) where the zeros occur. We give more details on this point in Section 5.

A first-order approximation reads

$$P_n[z(n+m)] \sim -(-1)^n n! e^{-nA} n^{-1/3} f_0 e^{-2\pi i/3} \text{Ai}(\eta n^{2/3} e^{-2\pi i/3}), \tag{3.7}$$

where

$$f_0 = \frac{1}{2}[f(\sqrt{\eta}) + f(-\sqrt{\eta})]$$

with f given in (3.6).

3.1. The condition for the zeros

We compare the condition for the location of the zeros of the quantities $P_n, Q_m, E_{n,m}$ as given in [11] with the condition that follows from the uniform Airy-type asymptotic approximation. Saff and Varga introduce the quantity

$$w_\sigma(z) = \frac{4\sigma^{\sigma/1+\sigma} z e^{g_\sigma(z)}}{(1 + \sigma)[1 + z + g_\sigma(z)]^{2/1+\sigma}[1 - z + g_\sigma(z)]^{2\sigma/1+\sigma}}, \quad 0 < \sigma < \infty, \tag{3.8}$$

where $g_\sigma(z)$ is defined in (3.3). Then the zeros of the three quantities $P_n, Q_m, E_{n,m}$ occur along curves in the z -plane defined by

$$|w_\sigma(z)| = 1. \tag{3.9}$$

By using the saddle points w^\pm defined in (3.3), a straightforward computation shows that

$$(1 + \sigma) \ln w_\sigma(z) = -\frac{4}{3}\eta^{3/2} - \sigma \ln(-1), \tag{3.10}$$

where $\frac{4}{3}\eta^{3/2}$ is defined in (3.6). The condition (3.9) can be read as: $\ln w_\sigma(z)$ is purely imaginary. So an equivalent formulation of (3.9) reads: $\eta^{3/2}$ is purely imaginary, i.e. the phase of η is $\pm\pi$ or $\pm\frac{1}{3}\pi$. In other words, η is located on the rays where the zeros occur of $\text{Ai}(z), \text{Ai}(e^{\pm 2\pi i/3}z)$.

3.2. An approximation of the zeros near z^+

We show how to obtain an asymptotic approximation of the zeros of $P_n[z(n+m)]$ near z^+ . The simpler case when $n=m$ is shortly discussed in [5]. In Section 4.2 an approximation of all zeros will be given. The Airy function $\text{Ai}(z)$ has zeros at the negative axis; let a_s denote these zeros. Then the main approximant in (3.7) has zeros at

$$\eta_s = n^{-2/3} e^{2\pi i/3} a_s, \quad s = 1, 2, 3, \dots$$

The corresponding z -values follow from inverting the relation between η and z given in (3.6). The first zeros (s small) give small values of η_s , that is, values z_s near z^+ . We expand

$$\eta = c_1(z - z^+) + c_2(z - z^+)^2 + \dots, \tag{3.11}$$

and try to find c_1, c_2, \dots . From (3.6) it follows by differentiating with respect to z (after straightforward and lengthy calculations):

$$2z\sqrt{\eta}\eta' = -(1 + \sigma)g_\sigma(z). \tag{3.12}$$

Squaring this equation and substituting (3.11), we obtain

$$4(z^+)^2 c_1^3 = (z^+ - z^-)(1 + \sigma)^2, \quad c_1^3 = i \frac{\sin \frac{1}{2}\theta}{\cos^3 \frac{1}{2}\theta} e^{-2i\theta},$$

where we use the relation between σ and θ given after (3.3). The cubic root gives three possibilities:

$$c_1 = e^{i(2\pi/3 + \pi/6 - 2i\theta/3)} \frac{\sin^{1/3} \frac{1}{2}\theta}{\cos \frac{1}{2}\theta}, \quad \varepsilon = -1, 0, 1.$$

The proper choice of ε follows from comparing this value of the coefficient with the one that follows from expanding the arctanh function in (2.5), where $\sigma = 1$ and $\theta = \frac{1}{2}\pi$, near $z = 1$ which gives

$$\eta = 2^{1/3}(1 - z)[1 + \mathcal{O}(1 - z)], \quad z \rightarrow 1$$

(observe that in Section 2 $P_n(2izn)$ is considered). This gives

$$z_s \sim z^+ - a_s e^{5\pi i/6 + 2i\theta/3} n^{-2/3} \frac{\cos \frac{1}{2}\theta}{\sin^{1/3} \frac{1}{2}\theta}, \quad n \rightarrow \infty. \tag{3.13}$$

When $\theta = \frac{1}{2}\pi$, $\sigma = 1$ this gives

$$z_s \sim i - a_s 2^{-1/3} e^{7\pi i/6} n^{-2/3},$$

which confirms the expression for the first zeros of $P_n(2izn)$ obtained in [5, Eq. (2.14)] when we turn that result over an angle $\frac{1}{2}\pi$.

Approximation (3.13) for the zeros of $P_n[z(n+m)]$ is valid for small values of s . The zeros of $Q_m[z(n+m)]$ follow from multiplying the second term in the right-hand side of (3.13) by $e^{2\pi i/3}$, those of $E_{n,m}[z(n+m)]$ from multiplying this term by $e^{-2\pi i/3}$.

For a recent discussion on how to obtain approximations of zeros of Airy-type asymptotic expansions, including order estimates of the remainders, we refer to [10].

4. More on Airy-type expansions

We first show how to obtain higher-order Airy-type approximations for integrals of a certain standard form.

4.1. Complete asymptotic expansions

We consider

$$F_n(\eta) := \frac{1}{2\pi i} \int_{\mathcal{C}} e^{n(\frac{1}{3}\zeta^3 - \eta\zeta)} f(\zeta) d\zeta, \tag{4.1}$$

where \mathcal{C} is a contour running from $\infty \exp(-\frac{1}{3}\pi i)$ to $\infty \exp(\frac{1}{3}\pi i)$, through the saddle point at $\zeta = \sqrt{\eta}$. We use the Bleistein method for obtaining a complete asymptotic expansion (this method was first given in [2] for a different class of integrals).

We define two sequences of functions $\{f_k\}, \{g_k\}$, $k = 0, 1, 2, \dots$ by writing

$$f_k(\zeta) = A_k - B_k \zeta + (\zeta^2 - \eta)g_k(\zeta), \quad f_{k+1}(\zeta) = -\frac{d}{d\zeta} g_k(\zeta), \tag{4.2}$$

with $f_0 = f$ and A_k, B_k following from substitution of $\zeta = \pm\sqrt{\eta}$. We have

$$A_k = \frac{1}{2}[f_k(\sqrt{\eta}) + f_k(-\sqrt{\eta})], \quad B_k = -\frac{1}{2\sqrt{\eta}}[f_k(\sqrt{\eta}) - f_k(-\sqrt{\eta})]. \tag{4.3}$$

By substituting $f(\zeta) = f_0(\zeta)$ of (4.2) into (4.1) and integrating N -times by parts we obtain

$$F_n(\eta) = \text{Ai}(\eta n^{2/3}) \sum_{k=0}^{N-1} \frac{A_k}{n^{k+1/3}} + \text{Ai}'(\eta n^{2/3}) \sum_{k=0}^{N-1} \frac{B_k}{n^{k+2/3}} + \varepsilon_N(\eta, n), \tag{4.4}$$

where

$$\varepsilon_N(\eta, n) = \frac{1}{n^N} \frac{1}{2\pi i} \int_{\mathcal{C}} e^{n(\frac{1}{3}\zeta^3 - \eta\zeta)} f_N(\zeta) d\zeta,$$

where $\text{Ai}'(z)$ is the derivative of the Airy function. If f is analytic in a certain domain of the complex plane, the functions f_k are, by inheritance, analytic functions in the same domain. For

proving that (2.4) gives a uniform asymptotic expansion as $n \rightarrow \infty$ (in particular, uniformly valid in a neighborhood of $\eta = 0$), we need estimates of $\varepsilon_N(\eta, n)$ in a neighborhood of \mathcal{C} . In the cases considered in this paper the parameters z and η are complex. For describing the zeros of P_n and Q_m z and η are restricted to compact sets, but the two infinite strings of zeros of $E_{n,m}$ extend to infinity.

Proofs for the asymptotic nature of uniform Airy-type expansions of integrals are considered in several places in the literature; for instance, see [8, 15]. In [6] a new method for representing the remainder and coefficients in Airy-type expansions of integrals is given. This approach gives a general method for extending the domain of the saddle-point parameter (η in the integral in (4.1)) to unbounded domains. A basic assumption for proving the validity of the uniform expansion in a unbounded domain, say $\eta \in \Delta$, is that the singularities of the function f should remain at a certain distance from the saddle points at $\pm\sqrt{\eta}$. To be more precise, let

$$\rho(\eta) = \min\{|\zeta \pm \sqrt{\eta}| \mid \zeta \text{ is a singularity of } f(\zeta)\}.$$

Then the assumption is $\rho(\eta) > |\eta|^\kappa$, $\eta \in \Delta$, where the constant κ should be larger than $-\frac{1}{2}$. We discuss later this property for the integrals considered in this paper.

4.2. Asymptotic expansions of the zeros

We first consider the expansion of the zeros of a function $W_n(\eta)$ having the asymptotic expansion

$$W_n(\eta) \sim \text{Ai}(\eta n^{2/3}) \sum_{k=0}^{\infty} \frac{A_k(\eta)}{n^k} + \text{Ai}'(\eta n^{2/3}) \sum_{k=0}^{\infty} \frac{B_k(\eta)}{n^{k+1/3}}. \tag{4.5}$$

We write $\eta = \alpha + \varepsilon$, where $\alpha = n^{-2/3} a_s$, with a_s is a zero of the Airy function $\text{Ai}(z)$. We write

$$W_n(\eta) = \sum_{m=0}^{\infty} \frac{\varepsilon^m}{m!} W_n^{(m)}(\alpha) = 0 \tag{4.6}$$

and obtain expansions for the derivatives from (4.5), i.e., by using $\text{Ai}''(z) = z \text{Ai}(z)$,

$$\frac{d^m}{d\eta^m} W_n(\eta) \sim n^m \left[\text{Ai}(\eta n^{2/3}) \sum_{k=0}^{\infty} \frac{A_k^m(\eta)}{n^k} + \text{Ai}'(\eta n^{2/3}) \sum_{k=0}^{\infty} \frac{B_k^m(\eta)}{n^{k+1/3}} \right],$$

where $A_k^0(\eta) = A_k(\eta)$, $B_k^0(\eta) = B_k(\eta)$ and, for $m = 1, 2, \dots$,

$$\begin{aligned} A_k^m(\eta) &= \eta B_k^{m-1}(\eta) + \frac{d}{d\eta} A_{k-1}^{m-1}(\eta), \\ B_k^m(\eta) &= A_k^{m-1}(\eta) + \frac{d}{d\eta} B_{k-1}^{m-1}(\eta); \end{aligned} \tag{4.7}$$

the functions with negative lower index are zero. Hence,

$$\frac{d^m}{d\eta^m} W_n(\alpha) \sim n^{m-1/3} \text{Ai}'(a_s) \sum_{k=0}^{\infty} \frac{B_k^m(\alpha)}{n^{k+1/3}},$$

and substituting this expansion in (4.6), we obtain the asymptotic equality

$$\sum_{k=0}^{\infty} \frac{B_k(x)}{n^k} + n\epsilon \sum_{k=0}^{\infty} \frac{B_k^1(x)}{n^k} + \frac{n^2 \epsilon^2}{2!} \sum_{k=0}^{\infty} \frac{B_k^2(x)}{n^k} + \frac{n^3 \epsilon^3}{3!} \sum_{k=0}^{\infty} \frac{B_k^3(x)}{n^k} + \dots \sim 0. \tag{4.8}$$

We try to find an expansion

$$\epsilon \sim \frac{x_1}{n} + \frac{x_2}{n^2} + \frac{x_3}{n^3} + \dots$$

Substituting this in (4.8), we obtain for x_1 the relation

$$B_0(x) + \frac{x_1}{1!} B_0^1(x) + \frac{x_1^2}{2!} B_0^2(x) + \frac{x_1^3}{3!} B_0^3(x) + \dots = 0.$$

Using the relations in (4.7), we obtain

$$B_0^m(\eta) = A_0^{m-1}(\eta) = \eta B_0^{m-2}(\eta) = \eta A_0^{m-3}(\eta) = \eta^2 B_0^{m-4} = \dots,$$

and for x_1 the equation

$$\cosh(\sqrt{x} x_1) B_0(x) + \frac{1}{\sqrt{x}} \sinh(\sqrt{x} x_1) A_0(x) = 0.$$

This gives

$$x_1 = -\frac{1}{\sqrt{x}} \operatorname{arctanh} \frac{\sqrt{x} B_0(x)}{A_0(x)}. \tag{4.9}$$

Higher-order coefficients x_j can be obtained, but we are satisfied with this first-order approximation. We infer that the function $W_n(\eta)$, having an asymptotic expansion as given in (4.5), for large values of n has a zero η_s associated with the zero a_s of the Airy function $\operatorname{Ai}(z)$, and we have found the approximation

$$\eta_s \sim x + \frac{x_1}{n}, \quad n \rightarrow \infty, \tag{4.10}$$

with $x = n^{-2/3} a_s$ and x_1 given in (4.9).

The above analysis is based on [7], where the method is used for obtaining asymptotic approximations of the zeros of Bessel functions of large order. In the Bessel function case odd powers of n are absent in the two series in (4.5). This gives a much simpler analysis for obtaining an expansion for the zeros.

4.3. Asymptotic expansions of the zeros of $P_n, Q_n, E_{n,m}$

When we use the above method for the quantity $E_{n,m}[z(n+m)]$, which has an expansion of the form (4.5), we have to calculate the zero z_s after having obtained the value η_s in (4.10). The corresponding z -value can be written as

$$z_s = z_s(\eta_s) = z_s(x + \epsilon) = z_s(x) + \frac{\epsilon}{1!} z_s'(x) + \frac{\epsilon^2}{2!} z_s''(x) + \dots = z_s(x) + \frac{z_s'(x) x_1}{n} + \mathcal{O}(n^{-2}), \tag{4.11}$$

where $z_s(x)$ follows from inverting the relation between η and z given in (3.6), with η replaced by x . After calculating $z_s(x)$ it is not difficult to obtain $z'_s(x)$, because from (3.12) it follows that

$$(1 + \sigma)g_\sigma(\eta) \frac{dz}{d\eta} = -2z\eta. \tag{4.12}$$

When we denote the infinite set of zeros of $E_{n,m}[z(n+m)]$ in the upper half-plane by $e_{n,m,s}$, we obtain the approximation

$$e_{n,m,s} = (n+m) \left[z_s(x) + \frac{z'_s(x) \alpha_1}{n} + \ell(n^{-2}) \right], \quad s = 1, 2, 3, \dots, \tag{4.13}$$

where α_1 is given in (4.9). This approximation holds uniformly with respect to s . There is a conjugate set of zeros $\bar{e}_{n,m,s}$ in the lower half-plane.

From (3.7) we see that $P_n[z(n+m)]$ has a complete expansion in terms of Airy functions with argument $\eta n^{2/3} e^{-2\pi i/3}$. It is not difficult to verify that in this case an approximation for the zeros is given by (4.10) with x replaced by $e^{2\pi i/3} x$ and α_1 evaluated as in (4.9) with this new value of x . An approximation for the corresponding z -value can then be obtained as in (4.11). For $Q_m[z(n+m)]$ the quantity x should be replaced by $e^{-2\pi i/3} x$.

The quantity α_1 used in the approximation of the zeros is given in (4.9). To use it we need the coefficients A_0, B_0 defined in (4.3) with f defined in (3.6). The quantities $f(\pm\sqrt{\eta})$ follow from a similar analysis as used for (2.11). We have

$$f(\sqrt{\eta}) = \frac{(4\eta)^{1/4}}{\sqrt{(1+\sigma)g_\sigma(z)w^+(w^++1)}}, \quad f(-\sqrt{\eta}) = \frac{(4\eta)^{1/4}}{\sqrt{(1+\sigma)g_\sigma(z)w^-(w^-+1)}},$$

where

$$w^+(w^++1) = \frac{1 - z \cos \theta + g_\sigma(z)}{2z^2}, \quad w^-(w^-+1) = \frac{1 - z \cos \theta - g_\sigma(z)}{2z^2}.$$

It follows that

$$\begin{aligned} -\frac{\sqrt{\eta}B_0(\eta)}{A_0(\eta)} &= \frac{f(\sqrt{\eta}) - f(-\sqrt{\eta})}{f(\sqrt{\eta}) + f(-\sqrt{\eta})} \\ &= \frac{\sqrt{w^-(w^-+1)} - \sqrt{w^+(w^++1)}}{\sqrt{w^-(w^-+1)} + \sqrt{w^+(w^++1)}} \\ &= e^{-i\theta} \sqrt{\frac{z - e^{i\theta}}{z - e^{-i\theta}}} \end{aligned}$$

and (4.9) becomes in this case

$$\alpha_1 = \frac{1}{\sqrt{x}} \operatorname{arctanh} e^{-i\theta} \sqrt{\frac{z_s(x) - e^{i\theta}}{z_s(x) - e^{-i\theta}}}.$$

5. More details on the cubic transformation (3.4)

The mapping $w \rightarrow \zeta(w)$ defined in (3.4) is singular at the points $w=0$ and $w=1$. These points are mapped into infinity. It is of interest to locate finite singularities of the mapping that are mapped to finite points in the ζ -plane. The singular points of the conformal mapping follow from the zeros of $d\zeta/dw$, see (3.6). The candidates are the saddle points w^\pm , but these are regular points because of the vanishing of $\eta - \zeta^2$ at the corresponding points $\pm\sqrt{\eta}$ in the ζ -plane. Less obvious candidates are the points outside the principal sheets of the logarithms occurring in $\phi(w)$. For instance, the derivative $d\zeta/dw$ again vanishes at the points $w^\pm e^{2\pi ik}$, $k = \pm 1, \pm 2, \dots$, and these points are not mapped to the points $\pm\sqrt{\eta}$ in the ζ -plane, because of $\ln w$ in $\phi(w)$. The term $\ln(w + 1)$ also gives rise to singular points.

Putting $w = w^\pm e^{2\pi ik}$, $k = \pm 1, \pm 2, \dots$ into (3.2) we obtain

$$\phi(w^\pm e^{2\pi ik}) = (1 + \sigma)w^\pm + \ln w^\pm + 2\pi ik + \sigma \ln(w^\pm + 1)$$

which reduces to $2\pi ik \pm \frac{2}{3}\eta^{3/2} + A$. The corresponding ζ -values can be obtained from the equation

$$2\pi ik \pm \frac{2}{3}\eta^{3/2} = -\frac{1}{3}\zeta^3 + \eta\zeta. \tag{5.1}$$

For example, when $z = 1.75i$, $\sigma = 1$, we have $\eta = -0.796\dots$ and $\eta^{3/2} = -0.710\dots i$. It follows that (5.1) has solutions on the imaginary axis. For $k = \pm 1$ we obtain the solutions $\zeta = \pm 4.846\dots i$. These points are singular points of the mapping (3.4). For the values of z, σ in this example the saddle points in the ζ -plane occur at $\pm\sqrt{\eta} = \pm 0.892\dots i$.

The possibility of constructing a valid uniform Airy-type expansion, as given in the previous section, depends on the regularity of the function $f(\zeta)$ in (4.1) in the neighborhood of the saddle points at $\pm\sqrt{\eta}$ and the growth of f along the contours of steepest descent. Most important is the regularity of f near the saddle points. In the above example we see saddle points at $\pm 0.892\dots i$ and nearby singularities at $\pm 4.846\dots i$ (other singularities in this example are at larger distances from the saddle points). The growth of f along the saddle point contours is at most of algebraic nature (see (3.6)).

When z runs through compact sets of the half-plane $\Im z > 0$, the singularities in the ζ -plane are bounded away from the saddle points $\pm\sqrt{\eta}$. For $z \rightarrow 0$ and $z \rightarrow \infty$ (this is, in particular, important for locating the zeros of $E_{n,m}(z)$), the singularities approach the saddle points. This can be seen as follows. We scale ζ by introducing $\chi = \zeta/\sqrt{\eta}$. Then (5.1) becomes

$$\chi - \frac{1}{3}\chi^3 = \pm \frac{2}{3} + 2\pi ik\eta^{-3/2}.$$

When η is large solutions occur near $\chi = \pm 1$ satisfying $\chi = \pm 1 + \mathcal{O}(\eta^{-3/4})$. It follows that solutions in the ζ -plane satisfy

$$\zeta = \pm\sqrt{\eta} + \mathcal{O}(\eta^{-1/4}), \quad \eta \rightarrow \infty.$$

We see that the distance between the singularities and the saddle points is $\mathcal{O}(\eta^{-1/4})$ as η becomes large. According to theorems in Section 5 of [6] we can accept distances of order $\eta^{-\theta}$ with $\theta > -\frac{1}{2}$. In the present case we have $\theta = -\frac{1}{4}$, which is safe enough. We conclude that an expansion as in (4.1) can be constructed for all points z with $\Im z \geq 0$ (and, in fact, in a larger domain, but that is not relevant here).

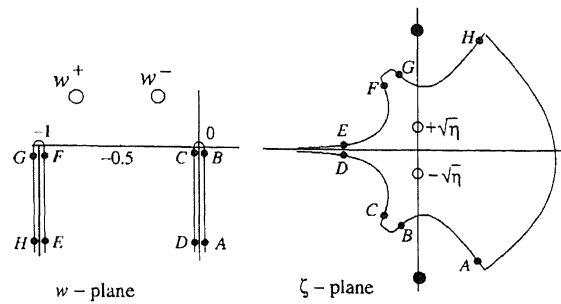


Fig. 4. Geometrical details of the mapping (3.4) with corresponding points in both planes. The black dots on the imaginary axis are singularities at $\zeta = \pm 4.846\dots i$.

In Fig. 4 we show geometrical components of the mapping in (3.4) for $\sigma=1, z=1.75i$. We exclude small neighborhoods of the branch cuts from 0 to $-\infty$ and from -1 to $-\infty$ and give corresponding points in both planes. The arc from H to A in the ζ -plane corresponds to a large circular arc in the w -plane from H to A , encircling the saddle points w^\pm . The points B, C and F, G tend to infinity in the ζ -plane, with $\arg \zeta = \mp \frac{2}{3}\pi$, as the corresponding points tend to 0 and -1 in the w -plane.

From the pictures it follows that the mapping is one-to-one on the boundary of the domain in the w -plane that lies outside the thin neighborhoods of the branch cuts. Because the mapping is analytic inside this domain and on the boundary, the mapping is univalent inside the domain (see [13, p. 201]).

The black dots on the imaginary axis are singularities at $\zeta = \pm 4.846\dots i$ corresponding to the points $w^\pm e^{\pm 2\pi i}$, which are outside the principal sheet of $\ln w$. For values of z on the positive imaginary axis this principal sheet is defined by $-\frac{1}{2}\pi < \arg w < \frac{3}{2}\pi$.

6. Numerical verification of the expansions for the zeros

In this section, we give more details on the computational aspects of the asymptotic estimate given in (4.13), and we give information on the singularities of η defined in (3.6) as a function of z .

For the expansion of $e_{n,m,s}$ given in (4.13) we claimed that it holds for all zeros in the upper plane. We can verify this by computing numerically the zeros of $E_{n,m}[z(n+m)]$ and compare the results with the two-term expansion in (4.13). In the diagonal case $n=m$ we can compare the zeros of $E_{n,m}[z(n+m)]$ with those of the Bessel function $J_{n+1/2}(-izn)$ since

$$E_{n,n}(2iz) = (-i)(2z)^n \sqrt{2\pi z} e^{-iz} J_{n+1/2}(z);$$

see (2.1) in [5]. The zeros of the J -Bessel function are easily computed, also when the order is large.

When we take $n=31$, the first zero of $J_{n+1/2}(-izn)$ on the positive imaginary axis has the value $z = 1.215727\dots i$ and the zero of $E_{n,m}(2zn)$ computed with (4.13), with $s=1$, has the value $1.2157877\dots i$, which gives an approximation with five corresponding digits (relative precision:

0.000049). The accuracy improves steadily for the larger zeros. For $s = 30$ we obtain $4.4957504\dots i$ and $4.4957801\dots i$, for the numerical and asymptotic values, respectively, with relative precision 0.0000066.

For the zeros of the polynomials P_n and Q_m we can use the same approximation given in (4.13) (with modifications as explained after (4.13)). When $n = m = 31$ there are 15 complex zeros for each polynomial in the upper half-plane and one real zero. The zero of P_n closest to $z = i$ has the value $-0.154582\dots + 0.916323\dots i$ (computed by Maple), and the approximation based on (4.13) gives $-0.154579\dots + 0.916388\dots i$ (which gives a relative precision of 0.00007). The real zero of P_n has the value $-0.673442\dots$, whereas (4.13) gives $-0.673433 + 0.000017\dots i$, which gives a relative precision of 0.00017, mainly due to the imaginary part; the real part has a relative precision of 0.000012, which is better than that of the first zero.

By inspecting more numerical results it follows that this time the zeros farther from $z = i$ become less accurate (as they approach the real axis). Although we need only $\lfloor \frac{1}{2}(n+1) \rfloor$ zeros for the polynomials (the other ones follow from conjugation), it is not as satisfactory as in the case of $E_{n,n}(2zn)$, and we will explain what is going wrong.

First we observe that, apparently, we have two possibilities for computing all n zeros of P_n :

- by using (4.13) for $s = 1, 2, \dots, n$;
- by using (4.13) for $s = 1, 2, \dots, \lfloor \frac{1}{2}(n+1) \rfloor$ and the remaining ones by using conjugation.

In addition to this we observe that we can continue the computations beyond $s = n$, because the Airy function has an infinite number of zeros. To explain this latter point, we remark that an approximation as given in (3.7) can also be used for noninteger values of n (with proper interpretation of P_n and $(-1)^n n!$). The integrals in (1.1)–(1.3) define functions for general complex values of n and m , and those functions (for instance, the Hankel functions in (2.1) in [4] (2.1) when $n = m$) have an infinite number of zeros, unless n is an integer, when they have exactly n zeros; see also [1, p. 373].

Also, when n is not an integer, the integrals in (1.1)–(1.3) define many-valued functions, and an appropriate choice of a branch cut for the generalized function P_n is the negative real axis. When we compute more than the first-half of the zeros of this P_n we have to interpret these zeros as lying outside the principal sector, i.e., with $\arg z > \pi$. When n is an integer these $\lfloor \frac{1}{2}n \rfloor$ zeros are exactly the conjugates of those in the upper half-plane.

6.1. Singularities of η as function of z

Another point is that the quantity η defined in (3.6) becomes singular at $z = e^{-i\theta}$. Recall that we assumed that η vanishes at the point $z = e^{i\theta}$ and is analytic at this point. At $z = e^{-i\theta}$ we see from (3.3) that $w^+ = w^-$ and from (3.6) that η vanishes again. However, this is false in general: the vanishing of η at $z = e^{-i\theta}$ depends on the actual phase of z at this point.

When z follows the curve of the early zeros of P_n in the left-hand plane, this curve crosses the negative axis, and the values of w^+ and w^- are not equal when z arrives at $z = e^{-i\theta}$ (in fact, their phases are different). Consider again the diagonal case $n = m$, with $\theta = \frac{1}{2}\pi$. At $z = i = e^{\frac{1}{2}\pi i}$, we have $w^+ = w^-$, but when $z = -i = e^{\frac{3}{2}\pi i}$ we have $w^+/w^- = e^{-2\pi i}$.

In Fig. 5 we show the trajectories of the saddle points w^\pm (defined in (3.3)) when z runs through the zeros of P_n with $n = m = 31$, starting near $z = i$ and ending at $z = -i = e^{\frac{3}{2}\pi i}$, with all zeros located

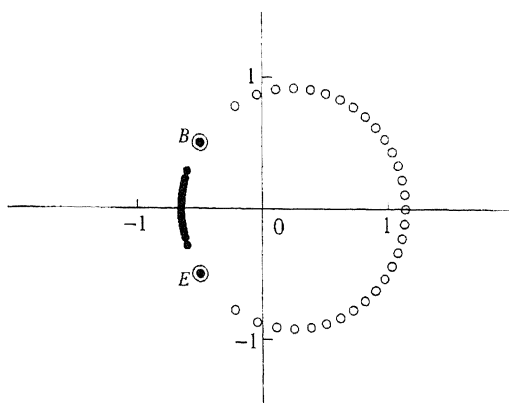


Fig. 5. Trajectories of the saddle points w^+ (open dots) and w^- (black dots) when z runs through the zeros of P_n , with $n = m = 31$. At B and E the saddle points coincide when $z = \pm i$.

in the half-plane $\Re z < 0$. At B and E the saddle points coincide (when $z = \pm i$). The saddle point w^+ describes a path from B to E , partly through the right-hand part of the plane, whereas w^- remains in the left-hand half-plane.

We infer from (3.6) that at $z = -i = e^{\frac{3}{2}\pi i}$ the parameter η is given by $\frac{2}{3}\eta^{3/2} = -2\pi i$, that is, $\eta = (3\pi/2)^{2/3}e^{-\pi i/3}$. Similarly, at $z = i = e^{-\frac{1}{2}\pi i}$ we have $\eta = (3\pi/2)^{2/3}e^{+\pi i/3}$. Now it is clear that, when we compute the zeros of P_n that lie in the lower half-plane $\Im z < 0$, the quantity η becomes singular as we approach $z = -i$. This makes an approximation as in (4.13) less accurate for these zeros, and it is better to use conjugation for the zeros of the polynomial P_n in $\Im z < 0$. Approximation (4.13) holds uniformly for all zeros of P_n located in $\Im z > 0$.

In the case that $n = m$, the relation for η given in (3.6) reads

$$\frac{2}{3}\eta^{3/2} = \ln \frac{1 + \sqrt{1 + z^2}}{-iz} - \sqrt{1 + z^2},$$

from which the role of the point $z = -i$ (with phases $\frac{3}{2}\pi$ and $-\frac{1}{2}\pi$) can be read off.

The relations given in (3.12) and (4.12) for $d\eta/dz$ also show that the mapping $z \rightarrow \eta(z)$ is not conformal when g_σ vanishes, except when $z = e^{i\theta}$. All points $z = e^{i\theta \pm 2k\pi i}$, $k = 1, 2, 3, \dots$ and $z = e^{-i\theta \pm 2k\pi i}$, $k = 0, 1, 2, \dots$ give singular points on the extended Riemann sheet of $\eta(z)$.

7. Concluding remarks

In a forthcoming paper on the quadratic Hermite–Padé Type I approximations associated with the exponential function the polynomials P_n , Q_m and R_s , having degrees n , m and s respectively, with P_n monic, that solve the approximation problem

$$E_{nms}(z) := P_n(z)e^{-2z} + Q_m(z)e^{-z} + R_s(z) = \mathcal{O}(z^{n+m+s+2}) \quad \text{as } z \rightarrow 0,$$

will be investigated for their asymptotic behavior and zero distribution. The quantities P_n , Q_m , R_s and E_{nms} have integral representations that are of a similar type as the ones given in (1.1)–(1.3).

More details can be found in [4], which is a preliminary study of this problem. Many properties of the quantities P_n , Q_m , R_s and E_{nms} are derived in that paper.

The present investigations have been done in order to become familiar with the more complicated methods from uniform asymptotics for obtaining information on the zeros of P_n , Q_m , R_s and E_{nms} of the Hermite–Padé case. We could have obtained the results of the present paper by considering the quantities defined in (1.1)–(1.3) as confluent hypergeometric functions, and by considering the differential equation for this class of special functions. In that way we might have used the powerful methods to obtain Airy-type expansions, including error bounds for the remainders, that are developed in [8]. However, for the Hermite–Padé case an approach based on linear differential equations seems not to be available.

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