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PARABOLIC CYLINDER FUNCTIONS: EXAMPLES OF ERROR BOUNDS FOR ASYMPTOTIC EXPANSIONS

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Several asymptotic expansions of parabolic cylinder functions are discussed and error bounds for remainders in the expansions are presented. In particular, Poincaré-type expansions for large values of the argument z and uniform expansions for large values of the parameter are considered. It is shown how expansions can be derived by using the differential equation, and, for a special case, how an integral representation can be used. The expansions are based on those given in Olver (1959) and on modifications of these expansions given in Temme (2000). Computer algebra techniques are used for obtaining representations of the bounds and for numerical computations.

Keywords: Parabolic cylinder functions; asymptotic expansions; error bounds for remainders; numerical evaluation of special functions.

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1. Introduction

The solutions of the differential equation

$$\frac{d^2y}{dz^2} - \left(\frac{1}{4}z^2 + a\right) y = 0 \tag{1.1}$$

are associated with the parabolic cylinder functions in harmonic analysis; see [10]. The solutions are called parabolic cylinder functions and are entire functions of z. Many properties are given in [3] and [1]; for applications to physics and many more properties see [2].

As in [3] and [1, Chapter 19], we denote two standard solutions of (1.1) by $U(a, z), V(a, z)$. Another well-known notation for the parabolic cylinder function is $D_\nu(z)$. The relationship between $D_\nu(z)$ and $U(a,z)$ is

$$D_\nu(z) = U\left(-\nu - \frac{1}{2}, z\right). \tag{1.2}$$

Wronskian relations for the solutions $U(a,z)$, $U(a,-z)$, $V(a,z)$ of (1.1) are:

$$U(a,z)V'(a,z) - U'(a,z)V(a,z) = \sqrt{2/\pi}, \tag{1.3}$$

$$U(a,z)\frac{dU(a,-z)}{dz} - U'(a,z)U(a,-z) = \frac{\sqrt{2\pi}}{\Gamma\left(a+\frac{1}{2}\right)}, \tag{1.4}$$

which shows that $U(a,z)$ and $V(a,z)$ are independent solutions of (1.1) for all values of a.

Other relations and connection formulae are

$$U(a,z) = \frac{\pi}{\cos^2 \pi a \Gamma\left(a+\frac{1}{2}\right)}\left[V(a,-z) - \sin \pi a\, V(a,z)\right], \tag{1.5}$$

$$\pi V(a,z) = \Gamma\left(\frac{1}{2}+a\right)\left[\sin \pi a\, U(a,z) + U(a,-z)\right], \tag{1.6}$$

$$\sqrt{2\pi}U(-a,iz) = \Gamma\left(\frac{1}{2}+a\right)\left[e^{-i\pi(\frac{1}{2}a-\frac{1}{4})}U(a,z) + e^{i\pi(\frac{1}{2}a-\frac{1}{4})}U(a,-z)\right], \tag{1.7}$$

$$U(a,z) = ie^{\pi i a}U(a,-z) + \frac{\sqrt{2\pi}}{\Gamma\left(a+\frac{1}{2}\right)}e^{\frac{1}{2}\pi i(a-\frac{1}{2})}U(-a,iz), \tag{1.8}$$

$$U(a,z) = -ie^{\pi i a}U(a,-z) + \frac{\sqrt{2\pi}}{\Gamma\left(a+\frac{1}{2}\right)}e^{-\frac{1}{2}\pi i(a-\frac{1}{2})U(-a,-iz)}. \tag{1.9}$$

In [5], an extensive collection of asymptotic expansions for the parabolic cylinder functions as $|a| \to \infty$ has been derived from the differential Eq. (1.1). The expansions are valid for complex values of the parameters and are given in terms of elementary functions and Airy functions. In [9], modified expansions are given, which have an extra feature that the expansions are also valid when a is fixed and z is large. The coefficients of the modified expansions can be generated by recursion formulas and are different from those of Olver's expansions.

When Olver published the paper [5], his later work on bounds for remainders in asymptotic expansions was not available, and, as he remarked in [8], the construction of error bounds for asymptotic expansions of the parabolic cylinder functions was an important problem to be considered. In this paper we discuss error bounds for the remainders of the standard Poincaré-type expansions of $U(a,z)$, and of some of the uniform expansions.

1.1. *Contents of the paper*

We summarize the results and give an overview of the structure of the paper. Section 1 gives the basic properties of the parabolic cylinder functions $U(a,z)$ and $V(a,z)$ that are used in this paper.

Section 2 gives the Poincaré-type expansions of $U(a,z)$ and $V(a,z)$ for large complex z, with a fixed. Section 2.1 gives the relation of $U(a,z)$ with the Whittaker function, and summarizes Olver's error bounds for the remainders in the expansion for the Whittaker function for several domains in the complex z plane. Section 2.2 discusses modifications or extensions of these domains by evaluating the variation $\mathcal{V}(f)$ along certain paths in a different way. Section 2.3 gives an application for the complementary error function erfc z, and tables comparing the exact upper bounds with remainders for z in the complex plane. It gives a different upper bound for a quantity used in Olver's estimate of $\mathcal{V}(t^{-n})$.

Section 3 gives the uniform asymptotic expansions for large real a with $t = z/(2\sqrt{|a|})$ as a real uniformity parameter. Several t intervals are considered. Section 3.1 derives expansions of $U(a,z)$ for large positive a and summarizes the method for obtaining the expansions by using the differential equation. Section 3.1.1 gives expansions and coefficients for $z \geq 0$. Section 3.1.2 gives expansions and coefficients for $z \leq 0$. Section 3.1.3 describes how to obtain error bounds for $z \geq 0$ and for $z \leq 0$, with tables indicating the accuracy of the estimates. Section 3.1.4 gives upper bounds for the variations of the coefficients ϕ_1, ϕ_2 and ϕ_3. Section 3.2 gives expansions for large negative a. This is the turning point case in which three t intervals can be indicated. Section 3.2.1 gives expansions of $U(a,z)$ and $V(a,z)$ for $t > 1$. Section 3.2.2 gives error bounds for the expansion of $U(a,z)$ for $t > 1$.

Section 4 gives two approaches for obtaining error bounds when a real integral representation of $U(a,z)$ is used. Section 4.1 gives the construction of a uniform expansion of $U(a,z)$ for large positive z, with $a \geq 0$; Section 4.2 describes a first method for deriving error bounds using real function values; Section 4.3 describes a method for deriving error bounds using complex function values and Cauchy-type integrals.

Section 5 discusses numerical aspects of computing the error bounds and the parabolic cylinder functions.

2. Poincaré-Type Expansions

These expansions are for large z and a fixed. They are given in [1] and derived in [11]. We have

$$U(a,z) \sim e^{-\frac{1}{4}z^2} z^{-a-\frac{1}{2}} \sum_{s=0}^{\infty} (-1)^s \frac{(a+\frac{1}{2})_{2s}}{s!(2z^2)^s}, \quad |\mathrm{ph}\, z| < \frac{3}{4}\pi, \tag{2.1}$$

$$V(a,z) \sim \sqrt{\frac{2}{\pi}} e^{\frac{1}{4}z^2} z^{a-\frac{1}{2}} \sum_{s=0}^{\infty} \frac{(-a+\frac{1}{2})_{2s}}{s!(2z^2)^s}, \quad |\mathrm{ph}\, z| < \frac{1}{4}\pi. \tag{2.2}$$

By using (1.8) and (1.9), the sector of validity of (2.1) can be modified, and compound expansions are obtained:

$$U(a,z) \sim e^{-\frac{1}{4}z^2} z^{-a-\frac{1}{2}} \sum_{s=0}^{\infty} (-1)^s \frac{(a+\frac{1}{2})_{2s}}{s!(2z^2)^s}$$

$$+ i\frac{\sqrt{2\pi}}{\Gamma(a+\frac{1}{2})} e^{-a\pi i} e^{\frac{1}{4}z^2} z^{a-\frac{1}{2}} \sum_{s=0}^{\infty} \frac{(-a+\frac{1}{2})_{2s}}{s!(2z^2)^s}, \quad \frac{1}{4}\pi < \text{ph } z < \frac{5}{4}\pi, \tag{2.3}$$

$$U(a,z) \sim e^{-\frac{1}{4}z^2} z^{-a-\frac{1}{2}} \sum_{s=0}^{\infty} (-1)^s \frac{(a+\frac{1}{2})_{2s}}{s!(2z^2)^s}$$

$$- i\frac{\sqrt{2\pi}}{\Gamma\left(a+\frac{1}{2}\right)} e^{a\pi i} e^{\frac{1}{4}z^2} z^{a-\frac{1}{2}} \sum_{s=0}^{\infty} \frac{\left(-a+\frac{1}{2}\right)_{2s}}{s!(2z^2)^s}, \quad -\frac{5}{4}\pi < \text{ph } z < -\frac{1}{4}\pi. \tag{2.4}$$

With these results, we also can obtain compound expansions for $V(a,z)$ for other sectors than the one given in (2.2).

2.1. *Error bounds of the expansions*

Bounds for remainders in the Poincaré-type expansion follow from [6],where results are given for Whittaker functions. The function $U(a,z)$ is a special case of this function. The relationship is

$$U(a,w) = 2^{-\frac{1}{2}a} w^{-\frac{1}{2}} W_{k,m}(z), \quad k = -\frac{1}{2}a, \quad m = \frac{1}{4}, \quad z = \frac{1}{2}w^2. \tag{2.5}$$

The asymptotic expansion for the Whittaker function reads

$$W_{k,m}(z) = z^k e^{-\frac{1}{2}z} \sum_{s=0}^{n-1} \frac{a_s}{z^s} + \epsilon_n(z), \quad a_s = (-1)^s \frac{(a+\frac{1}{2})_{2s}}{2^{2s}\, s!}, \quad n = 0,1,2,\ldots. \tag{2.6}$$

We introduce the following quantities. Let

$$\begin{aligned} &\kappa = |a|, \quad \sigma = \kappa |z|^{-1}, \quad \alpha = (1-\sigma)^{-1}, \quad \beta = \frac{1}{2} + \frac{1}{2}\sigma + \frac{1}{2}\sigma\alpha|z|^{-1}, \\ &\delta = \left|\frac{1}{4}a^2 + \frac{3}{16}\right| + \sigma\left(1 + \frac{1}{4}\sigma\right)\alpha^2, \end{aligned} \tag{2.7}$$

assuming that $\sigma < 1$. Then the remainder $\epsilon_n(z)$ of (2.6) and its derivative can be bounded as follows

$$\left.\begin{aligned} |\epsilon_n(z)| &\le \\ |\beta^{-1}\epsilon_n'(z)| &\le \end{aligned}\right\} 2\alpha \left| z^k e^{-\frac{1}{2}z} a_n \right| \mathcal{V}_p(t^{-n}) \exp\left[2\alpha\delta \mathcal{V}_p(t^{-1})\right], \tag{2.8}$$

where $\mathcal{V}(f)$ denotes the variational operator (see [7]),which for continuously differentiable functions in a real interval $[a, b]$ is defined by

$$\mathcal{V}_{a,b}(f) = \int_a^b |f'(x)|dx\,. \tag{2.9}$$

For a holomorphic function $f(z)$ in a complex domain, the variational operator along a smooth arc $\mathcal{C}$ parameterized by $z(\tau)$, $\alpha < \tau < \beta$, in which τ is the arc parameter and $z'(\tau)$ is continuous and nonvanishing in the closure of (α, β), we have

$$\mathcal{V}_{\mathcal{C}}(f) = \int_\alpha^\beta |f'[z(\tau)]z'(\tau)|\; d\tau. \tag{2.10}$$

Along a path $\mathcal{P}$ which is a finite chain of smooth arcs (of straight lines, for example) $\mathcal{V}_{\mathcal{P}}$ can be defined as the sum of the contributions from the arcs.

In the bounds given in (2.8), the path $\mathcal{P}$ links the point z $\big($with ph $z \in (-\frac{3}{2}\pi, \frac{3}{2}\pi)\big)$ to $+\infty$, such that on $\mathcal{P}$ the condition is fulfilled that $\Re(t + a\ln t)$ is monotonic.

We consider the bounds in (2.8) for z in the sector $[-\pi, \pi]$, that is, for w used in (2.5) with $\Re w \geq 0$. For other values of w, the relations in (1.8) and (1.9) can be used for computing the function $U(a, w)$.

In [6], simple bounds are given for the variation $\mathcal{V}_{\mathcal{P}}(t^{-n})$ appearing in (2.8), for z in certain regions in the complex plane. In Fig. 1, we show these regions in the z-plane and corresponding regions in the w-plane; we only show the regions in $\Im_z \geq 0$, $\Im w \geq 0$, but they should be extended by including the conjugated parts.

The arc PQ is a circular arc, with radius 2κ; Q is the point $-\sqrt{3}\kappa + i\kappa$; S is the point $i\kappa$; the arc ST is a circular arc, with radius κ. As in (2.7) $\kappa = |a|$.

The region R_1 is the half-plane $\Re z \geq \kappa$; R_2 is the region above the curves VQ, QS, ST and the conjugated z-values; R_4 is the region with $|z| \geq 2\kappa$, $|\Im z| \leq \kappa$. The corresponding regions in the w-plane follow from $z = \frac{1}{2}w^2$.

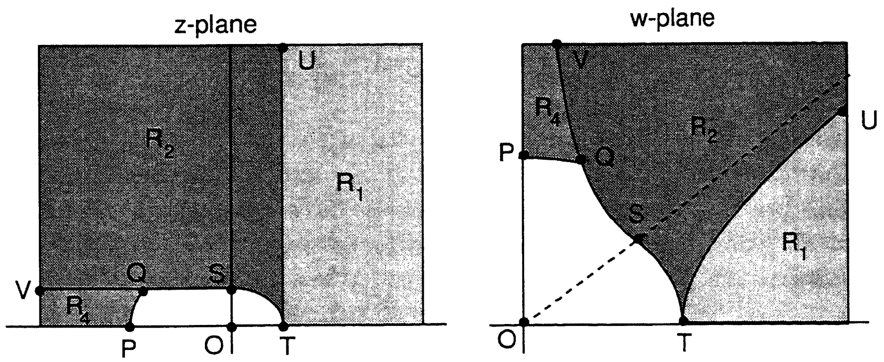

Fig. 1. The region R_1, R_2, and R_4 used for bounding the variation $\mathcal{V}_{\mathcal{P}}(t^{-n})$ appearing in (2.8).

The following upper bounds for $\mathcal{V}_{\mathcal{P}}(t^{-n})$ are derived in [6]:

$$\begin{array}{ll} |z|^{-n}, & z \in R_1, \\ \chi(n)|z|^{-n}, & z \in R_2, \\ \left[\chi(n) + \sigma v^2 n\right] v^n |z|^{-n}, & z \in R_4\,, \end{array} \tag{2.11}$$

where

$$\chi(n) = \frac{\sqrt{\pi}\,\Gamma\left(\frac{1}{2}n+1\right)}{\Gamma\left(\frac{1}{2}n+\frac{1}{2}\right)}, \quad v = \left(\frac{1}{2}+\frac{1}{2}\sqrt{1-4\sigma^2}\right)^{-\frac{1}{2}}. \tag{2.12}$$

For $\mathcal{V}_{\mathcal{P}}\left(t^{-1}\right)$ set $n=1$ in (2.11).

For $z \in R_4$, the quantities α, β, and δ of (2.7) should be modified: replace σ by $v\sigma$ and $|z|^{-1}$ by $v|z|^{-1}$.

For the parabolic cylinder function $U(a,w)$, these bounds are applicable if $|w|$ is large compared with $\sqrt{|a|}$. For example, if $w \in R_4$, then we need $|w| \geq 2\sqrt{|a|}$. However, if ω is not large compared with $\sqrt{|a|}$, then the asymptotic expansion does not make sense, and, hence, the condition $|w| \geq 2\sqrt{|a|}$ does not cause a restriction in the use of the asymptotic expansion.

2.2. *Are these domains optimal?*

We have used the same values as in [6] for showing the regions R_1, R_2, and R_4. When verifying Olver's analysis, we have found that the boundaries of the regions R_1 and R_2 can be modified.

2.2.1. *Extending the region R_1*

For R_1, we can use the condition $\Re z > \max[0, \Re(-a)]$. To verify this condition, let

$$a = u + iv = |a|e^{i\alpha}, \quad z = x + iy = re^{i\phi}. \tag{2.13}$$

In Olver's analysis, the path in the z-plane has to be selected such that along this path

$$F(x,y) = \Re(z + a\ln z) = x + \frac{1}{2}u\ln(x^2+y^2) - v\arctan(y/x) \tag{2.14}$$

is monotonic. Olver chose an optimal path with the constant argument ϕ. Substituting $y = x\tan\phi$ in $F(x,y)$, we find $dF/dx = (u+x)/x$. This is positive on the path when $\Re z > \max[0, \Re(-a)]$. One can also use a vertical path $x = x_0, y \geq y_0$ upwards, if $\phi \in (\alpha, \alpha+\pi)$. This follows from

$$\frac{dF(x_0,y)}{dy} = \frac{uy - vx_0}{x_0^2 + y^2}. \tag{2.15}$$

Similarly, one can use the vertical path downwards if $\phi \in (\alpha - \pi, \alpha)$. In Olver's approach vertical paths are not used.

2.2.2. *Extending the region R_2*

For R_2, the condition $\Im z > \max[0, \Im(-a)]$ can be used. We verify this by taking as region R_2 (as in Olver's approach) the domain with points $z_0 = x_0 + iy_0$ from which we can draw a half line with the equation $x_0 x + y_0 y = x_0^2 + y_0^2$. This line is perpendicular (at $z = z_0$) to the line from the origin to z_0. Another equation for the line is $y = y_0 - \frac{x_0}{y_0}(x - x_0)$. On this path we have

$$\frac{dF}{dx} = 1 + \frac{u(x_0^2 + y_0^2)}{y_0^2(x^2 + y^2)}(x - x_0) + \frac{v(x_0^2 + y_0^2)}{y_0(x^2 + y^2)}, \tag{2.16}$$

and we see that $dF/dx > 0$ at $z = z_0$ if $0 < -v < y_0$ or $v > 0, y_0 > 0$. With these conditions, we have $dF/dx > 0$ for all $x > x_0$. This explains why we can extend region R_2 to the domain where $\Im z > \max(0, \Im(-a))$.

2.3. *Application to the complementary error function*

We have applied these bounds for the case $a = \frac{1}{2}$, which corresponds to the complementary error function:

$$W_{-\frac{1}{4},\frac{1}{4}}(z) = \sqrt{\pi} z^{\frac{1}{4}} e^z \operatorname{erfc} \sqrt{z}\,. \tag{2.17}$$

We have computed

$$\rho = \frac{|\epsilon_n(z)|}{\epsilon_n^{(e)}(z)} \tag{2.18}$$

where $\epsilon_n(z)$ is the exact error (see (2.6)), $\epsilon_n^{(e)}(z)$ the estimated error (see (2.8)), for several values of n and $\theta = \operatorname{ph} z$ as given in Table 1. We observe that the ratio ρ is almost always less than $\frac{1}{3}$, and that in R_2, where $\theta = \frac{j}{8}\pi$ with $j = 4, 5, 6, 7$, the estimated error is quite large compared with the real error.

Table 1. Ratios $\rho = |\epsilon_n(z)|/\epsilon_n^{(e)}(z); z = re^{i\theta},\ r = 10$.

θ	$\frac{0}{8}\pi$	$\frac{1}{8}\pi$	$\frac{2}{8}\pi$	$\frac{3}{8}\pi$	$\frac{4}{8}\pi$	$\frac{5}{8}\pi$	$\frac{6}{8}\pi$	$\frac{7}{8}\pi$	$\frac{8}{8}\pi$
$n = 5$	0.29	0.30	0.31	0.34	0.13	0.15	0.18	0.25	0.34
$n = 10$	0.22	0.23	0.24	0.26	0.07	0.09	0.12	0.20	0.37
$n = 15$	0.18	0.18	0.19	0.21	0.05	0.06	0.08	0.12	0.19

The upper bound $\chi(n)$ of the variation (see (2.12)) introduced by Olver is not very sharp for certain values of the parameter. In his analysis, the estimate of the variation along a certain path follows from

$$\mathcal{V}_{\mathcal{P}}(t^{-n}) = \int_0^\infty \frac{n\,d\tau}{|z + \tau e^{i\phi}|^{n+1}} = \int_0^\infty \frac{n\,d\tau}{||z|e^{i(\theta-\phi)} + \tau|^{n+1}}\,, \tag{2.19}$$

Table 2. Ratios as in Table 1, now with variations $\mathcal{V}_{\mathcal{P}}(t^{-n})$ according to (2.21).

θ	$\frac{0}{8}\pi$	$\frac{1}{8}\pi$	$\frac{2}{8}\pi$	$\frac{3}{8}\pi$	$\frac{4}{8}\pi$	$\frac{5}{8}\pi$	$\frac{6}{8}\pi$	$\frac{7}{8}\pi$	$\frac{8}{8}\pi$
$n = 5$	0.29	0.30	0.31	0.34	0.38	0.42	0.43	0.41	0.32
$n = 10$	0.22	0.23	0.24	0.26	0.31	0.35	0.38	0.39	0.33
$n = 15$	0.18	0.18	0.19	0.21	0.25	0.28	0.29	0.27	0.17

where $\theta = \text{ph } z$ and $\phi \in [-\frac{1}{2}\pi, \frac{1}{2}\pi]$ is defined by $\cos\phi = \kappa/|z|$, where $\kappa = |a|$ is introduced in (2.7). The right-hand side of (2.19) is estimated by Olver as follows:

$$\int_0^\infty \frac{n\,d\tau}{||z|e^{i(\theta-\phi)} + \tau|^{n+1}} \le \int_0^\infty \frac{n\,d\tau}{(|z|^2 + \tau^2)^{\frac{1}{2}n+\frac{1}{2}}} = \frac{\chi(n)}{|z|^n}. \tag{2.20}$$

The right-hand side of (2.19) can be written as a Gauss hypergeometric function, and we find for the variation (along the same path $\mathcal{P}$)

$$\begin{aligned} \mathcal{V}_{\mathcal{P}}(t^{-n}) &= \frac{n}{|z|^n}\int_0^\infty \frac{d\tau}{(u^2 + 2\cos(\theta-\phi)u + 1)^{\frac{1}{2}n+\frac{1}{2}}} \\ &= \frac{1}{|z|^n}\,{}_2F_1\left(\frac{1}{2}n, \frac{1}{2}; \frac{1}{2}n + 1; \sin^2(\theta - \phi)\right). \end{aligned} \tag{2.21}$$

The value $\chi(n)$ follows from this expression when we replace the argument of the hypergeometric function by unity. With this new value of $\mathcal{V}_{\mathcal{P}}$, we re-computed the ratios of Table 1, and we give the new ratios in Table 2. We see that indeed the ratios become larger in the regions R_2 and R_4, except when $\theta = \pi$. That is, when we use (2.21), the estimates of the remainders become more realistic in these regions.

3. Uniform Expansions in Terms of Elementary Functions

We transform the differential Eq. (1.1) into a standard form and distinguish between the cases when there are no real turning points (when $a > 0$), and when there are two real turning points (when $a < 0$). For convenience, we consider real parameters.

3.1. *Positive a*

For $a > 0$, no oscillations occur on the real z-axis. In [5], expansions are given that cover all real z. We consider two different modifications, one for $z \ge 0$ and another one for $z \le 0$. These modifications are derived in [9], and we use the notation of that reference.

The function $U(a, z)$ is a solution of (1.1), and $w(t) = U\left(\frac{1}{2}\mu^2, \mu t\sqrt{2}\right)$ satisfies

$$\frac{d^2w}{dt^2} = \mu^4(t^2 + 1)w. \tag{3.1}$$

The function $W(t) = (t^2+1)^{\frac{1}{4}} U\left(\frac{1}{2}\mu^2, \mu t\sqrt{2}\right)$ is a solution of

$$\frac{d^2W}{d\widetilde{\xi}^2} = [\mu^4 + \psi(\widetilde{\xi})]w \tag{3.2}$$

where the relation between t and $\widetilde{\xi}$ is given by

$$\widetilde{\xi} = \frac{1}{2}t\sqrt{t^2+1} + \frac{1}{2}\ln[t + \sqrt{t^2+1}], \tag{3.3}$$

and $\psi(\widetilde{\xi})$ is given by

$$\psi(\widetilde{\xi}) = \frac{2-3t^2}{4(t^2+1)^3}. \tag{3.4}$$

Transformations of this kind are discussed in [7, Chapter 10]. The relation in (3.3) follows from

$$\frac{d\widetilde{\xi}}{dt} = \sqrt{t^2+1}, \quad \widetilde{\xi}(0) = 0, \tag{3.5}$$

which arises in a Liouville–Green transformation ([5, 7]).

The quantity $\widetilde{F}$, defined by

$$\widetilde{F} = e^{\mu^2\widetilde{\xi}}\, W, \tag{3.6}$$

is a solution of

$$\frac{d^2\widetilde{F}}{d\widetilde{\xi}^2} - 2\mu^2\frac{d\widetilde{F}}{d\widetilde{\xi}} - \psi(\widetilde{\xi})\widetilde{F} = 0. \tag{3.7}$$

It is convenient to introduce another parameter, $\widetilde{\tau}$, by writing

$$\widetilde{\tau} = \frac{1}{2}\left[\frac{t}{\sqrt{t^2+1}} - 1\right]. \tag{3.8}$$

We have

$$\frac{d\widetilde{\xi}}{d\widetilde{\tau}} = \frac{1}{8\widetilde{\tau}^2(1+\widetilde{\tau})^2}, \tag{3.9}$$

and Eq. (3.7) becomes in terms of $\widetilde{\tau}$:

$$16\widetilde{\tau}^2(\widetilde{\tau}+1)^2\frac{d^2\widetilde{F}}{d\widetilde{\tau}^2} + \left[32\widetilde{\tau}(2\widetilde{\tau}^2+3\widetilde{\tau}+1) - 4\mu^2\right]\frac{d\widetilde{F}}{d\widetilde{\tau}} + (20\widetilde{\tau}^2+20\widetilde{\tau}+3)\widetilde{F} = 0. \tag{3.10}$$

3.1.1. *The case $z \geq 0$*

We give an asymptotic expansion of the U-function for $a \to +\infty$ that holds uniformly for $z \geq 0$. We write

$$U\left(\frac{1}{2}\mu^2, \mu t\sqrt{2}\right) = \frac{e^{-\mu^2\widetilde{\xi}}}{\sqrt{2}\mu h(\mu)(t^2+1)^{\frac{1}{4}}}\widetilde{F}_\mu(\widetilde{\tau}) \tag{3.11}$$

where $\widetilde{F}_\mu(\widetilde{\tau})$ satisfies Eq. (3.10) and is expanded in the form

$$\widetilde{F}_\mu(\widetilde{\tau}) \sim \sum_{s=0}^{\infty}(-1)^s\frac{\phi_s(\widetilde{\tau})}{\mu^{2s}} \tag{3.12}$$

where

$$h(\mu) = 2^{-\frac{1}{4}\mu^2-\frac{1}{4}}e^{-\frac{1}{4}\mu^2}\mu^{\frac{1}{2}\mu^2-\frac{1}{2}} = 2^{-\frac{1}{2}}e^{-\frac{1}{2}a}a^{\frac{1}{2}a-\frac{1}{4}}. \tag{3.13}$$

Substituting (3.12) into (3.10) and prescribing

$$\phi_0(\tau) = 1, \quad \phi_s(0) = 0, \quad s \geq 1, \tag{3.14}$$

we find that the coefficients ϕ_s of (3.12) are polynomials in $\widetilde{\tau}$ of degree $3s$ and are given by the recursion relation

$$\phi_{s+1}(\tau) = -4\tau^2(\tau+1)^2\frac{d}{d\tau}\phi_s(\tau) - \frac{1}{4}\int_0^\tau\left(20u^2+20u+3\right)\phi_s(u)\,du. \tag{3.15}$$

This relation follows easily when (3.10) is written in the form

$$\mu^2\frac{d\widetilde{F}}{d\widetilde{\tau}} = 4\frac{d}{d\widetilde{\tau}}\left[\widetilde{\tau}^2(\widetilde{\tau}+1)^2\frac{d\widetilde{F}}{d\widetilde{\tau}}\right] + \frac{1}{4}(20\widetilde{\tau}^2+20\widetilde{\tau}+3)\widetilde{F}. \tag{3.16}$$

The term $h(\mu)$ given in (3.13) follows from (2.1) and from the conditions on ϕ_s given in (3.14).

The expansion in (3.12) corresponds to the expansion (11.10) given in [5]. Both Olver's and our expansions hold for large a, uniformly for all real z. But for negative values of z, we prefer a slightly different expansion that will be given in the next subsection. The expansions also hold in unbounded complex domains. For details, we refer the reader to [5]. Our expansions have a double asymptotic property: they also are valid for bounded a with z large, and when both parameters are large.

The first few coefficients of (3.12) are

$$\begin{aligned}
\phi_0(\tau) &= 1\,,\\
\phi_1(\tau) &= -\frac{\tau}{12}(20\tau^2+30\tau+9)\,,\\
\phi_2(\tau) &= \frac{\tau^2}{288}(6160\tau^4+18480\tau^3+19404\tau^2+8028\tau+945)\,,\\
\phi_3(\tau) &= -\frac{\tau^3}{51840}(27227200\tau^6+122522400\tau^5+220540320\tau^4\\
&\quad +200166120\tau^3+94064328\tau^2+20545650\tau+1403325)\,,
\end{aligned} \tag{3.17}$$

For the derivative, we have

$$U'\left(\frac{1}{2}\mu^2, \mu t\sqrt{2}\right) = -\frac{(1+t^2)^{\frac{1}{4}}\, e^{-\mu^2\widetilde{\xi}}}{2h(\mu)}\widetilde{G}_\mu(t), \quad \widetilde{G}_\mu(t) \sim \sum_{s=0}^{\infty}(-1)^s \frac{\psi_s(\widetilde{\tau})}{\mu^{2s}}, \quad (3.18)$$

where the coefficients $\psi_s(\tau)$ can be obtained by formal differentiation of (3.11) and (3.12). It follows that

$$\psi_s(\tau) = \phi_s(\tau) + 2\tau(\tau+1)(2\tau+1)\phi_{s-1}(\tau) + 8\tau^2(\tau+1)^2\frac{d\phi_{s-1}(\tau)}{d\tau}, \quad (3.19)$$

$s = 0, 1, 2, \ldots$. The first few coefficients are

$$\begin{aligned}
\psi_0(\tau) &= 1, \\
\psi_1(\tau) &= \frac{\tau}{12}(28\tau^2 + 42\tau + 15), \\
\psi_2(\tau) &= -\frac{\tau^2}{288}(7280\tau^4 + 21840\tau^3 + 23028\tau^2 + 9684\tau + 1215), \\
\psi_3(\tau) &= \frac{\tau^3}{51840}(304304000\tau^6 + 1369368000\tau^5 + 2467080000\tau^4 \\
&\quad + 2244942000\tau^3 + 1061223120\tau^2 + 234891900\tau + 16584750).
\end{aligned} \quad (3.20)$$

3.1.2. *The case* $z \le 0$

For negative z, we have

$$\begin{aligned}
U\left(\frac{1}{2}\mu^2, -\mu t\sqrt{2}\right) &= \frac{\sqrt{2\pi}}{\Gamma(\frac{1}{2}+\frac{1}{2}\mu^2)}\frac{h(\mu)e^{\mu^2\widetilde{\xi}}}{(1+t^2)^{\frac{1}{4}}}\widetilde{P}_\mu(t), \\
U'\left(\frac{1}{2}\mu^2, -\mu t\sqrt{2}\right) &= -\frac{\sqrt{\pi}\,\mu h(\mu)}{\Gamma\left(\frac{1}{2}+\frac{1}{2}\mu^2\right)}e^{\mu^2\widetilde{\xi}}(1+t^2)^{\frac{1}{4}}\,\widetilde{Q}_\mu(t),
\end{aligned} \quad (3.21)$$

where $\widetilde{\xi}$, $\widetilde{\tau}$, and $h(\mu)$ are defined in (3.3), (3.8), and (3.13), respectively, and

$$\widetilde{P}_\mu(t) \sim \sum_{s=0}^{\infty}\frac{\phi_s(\widetilde{\tau})}{\mu^{2s}}, \quad \widetilde{Q}_\mu(t) \sim \sum_{s=0}^{\infty}\frac{\psi_s(\widetilde{\tau})}{\mu^{2s}}. \quad (3.22)$$

Again, these expansions have a double asymptotic property: they are valid when a or t (or both) are large.

The functions $\widetilde{F}_\mu(t)$, $\widetilde{G}_\mu(t)$, $\widetilde{P}_\mu(t)$, and $\widetilde{Q}_\mu(t)$ satisfy the following exact relation:

$$\widetilde{F}_\mu(t)\widetilde{Q}_\mu(t) + \widetilde{G}_\mu(t)\widetilde{P}_\mu(t) = 2. \quad (3.23)$$

To obtain expansions for $V(a,z)$ and its derivative, the relation in (1.6) can be used.

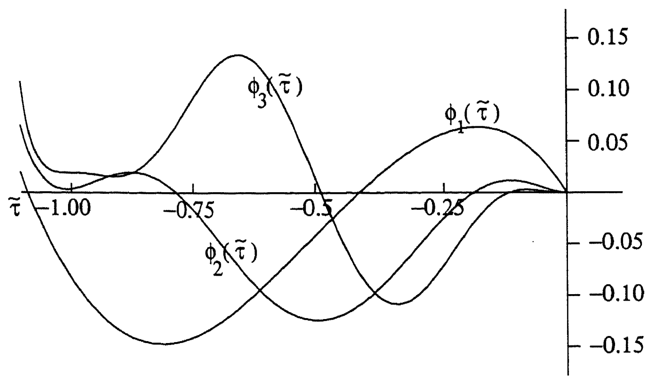

Fig. 2. Graphs of $\phi_s(\widetilde{\tau})$, $s = 1, 2, 3$, $\widetilde{\tau} \in [-1, 0]$.

3.1.3. *Error bounds of the expansions*

We apply [7, p. 366, Theorem 3.1] and write the expansion in (3.12) with a remainder. For $n = 0, 1, 2, \ldots$, we have

$$\widetilde{F}_\mu(t) = \sum_{s=0}^{n-1} (-1)^s \frac{\phi_s(\widetilde{\tau})}{\mu^{2s}} + \widetilde{R}_n(\mu, t)\,. \tag{3.24}$$

The remainder $\widetilde{R}_n(\mu, t)$ can be bounded as follows

$$|\widetilde{R}_n(\mu, t)| \le \exp\left[\frac{2\mathcal{V}_{\widetilde{\xi},\infty}(\phi_1)}{\mu^2}\right] \frac{\mathcal{V}_{\widetilde{\xi},\infty}(\phi_n)}{\mu^{2n}} \tag{3.25}$$

where we take into account that we consider positive t and μ (see also [7, p. 367, Exercise 3.1]).

We need the variation of the coefficients ϕ_s for $t \ge 0$, which corresponds with $\widetilde{\xi} \ge 0$ and $-\frac{1}{2} \le \widetilde{\tau} \le 0$; cf. (3.8). We have

$$\mathcal{V}_{\widetilde{\xi},\infty}(\phi_n) = \int_{\widetilde{\tau}}^{0} |\phi_n'(\tau)|\, d\tau\,. \tag{3.26}$$

For negative argument, the coefficients ϕ_s oscillate; see Fig. 2.

In Table 3, we show the ratios $|R_n(\mu, t)|/R_n^{(e)}(\mu, t)$ (with $n = 3$) where $R_n^{(e)}(\mu, t)$ is the right-hand side of (3.25). We see that the estimates for small values of t are much too large. An explanation is that for small t (that is, $\widetilde{\tau}$ close to $-\frac{1}{2}$), the variations in (3.26) are calculated over a larger interval than when t is large. Expansion (3.24) has a double asymptotic property, and large values of t are quite favorable for the expansion.

For $z \le 0$, we consider the remainder in the expansion of (3.22) and we write

$$\widetilde{P}_\mu(t) = \sum_{s=0}^{n-1} \frac{\phi_s(\widetilde{\tau})}{\mu^{2s}} + \widetilde{R}_n(\mu, t)\,. \tag{3.27}$$

Table 3. Ratios $|R_n(\mu,t)|/R_n^{(e)}(\mu,t)$; $z = 2t\sqrt{a}\,, n = 3$.

t	0.0	1.0	2.5	5.0	10	25	50
$a = 1$	.21493	.14455	.84677	.94186	.98360	.99728	.99932
$a = 5$	.06142	.43256	.96494	.98773	.99667	.99945	.99986
$a = 10$	.00343	.50123	.98214	.99382	.99833	.99973	.99993
$a = 50$	.04921	.56597	.99637	.99876	.99967	.99995	.99999
$a = 100$	.05601	.57478	.99818	.99938	.99983	.99997	.99999

Table 4. Ratios $|R_n(\mu,t)|/R_n^{(e)}(\mu,t)$; $z = -2t\sqrt{a}\,, n = 3$.

t	0.0	1.0	2.5	5.0	10	25	50
$a = 1$	.29041	.04469	.87352	.76079	.72513	.71493	.71347
$a = 5$	.17780	.02071	.96996	.94637	.93771	.93509	.93471
$a = 10$	.12433	.01817	.98467	.97279	.96835	.96700	.96680
$a = 50$	.07476	.01644	.99689	.99449	.99359	.99331	.99327
$a = 100$	.06829	.01624	.99844	.99724	.99679	.99665	.99663

In the present case, we have the bound

$$|\widetilde{R}_n(\mu,t)| \le \exp\left[\frac{2\mathcal{V}_{-\infty,\widetilde{\xi}}(\phi_1)}{\mu^2}\right]\frac{\mathcal{V}_{-\infty,\widetilde{\xi}}(\phi_n)}{\mu^{2n}} \tag{3.28}$$

where

$$\mathcal{V}_{-\infty,\widetilde{\xi}}(\phi_n) = \int_{-1}^{\widetilde{\tau}} |\phi_n'(\tau)|\,d\tau\,. \tag{3.29}$$

In Table 4, we show the ratios $|R_n(\mu,t)|/R_n^{(e)}(\mu,t)$ (with $n = 3$) where in the present case $R_n^{(e)}(\mu,t)$ is the right-hand side of (3.28). We see that, in general, the ratios are smaller than when $z \ge 0$. An explanation is that the variations in (3.29) include the contributions from the interval $\left[-1,-\frac{1}{2}\right]$ (corresponding with the $\widetilde{\xi}$ interval $(-\infty,0]$). The parameter $\widetilde{\tau}$ remains in the interval $\left[-\frac{1}{2},0\right]$, however, when $t \ge 0$ $(z \le 0)$.

3.1.4. *Upper bounds for the variations of $\phi_s(\widetilde{\tau})$*

The variations of the coefficients $\phi_s(\widetilde{\tau})$ used in (3.26) and (3.29) can be computed by numerical quadrature of the integrals, but for real values, it is convenient to use the zeros of the polynomials $\phi_s'(\widetilde{\tau})$. For example, $\phi_1'(\widetilde{\tau})$ has zeros at $t_1 = -0.816$ and $t_2 = -0.184$. Hence, for $\widetilde{\tau} \in \left[-\frac{1}{2},0\right]$, the variation in (3.26) follows from

$$\mathcal{V}_{\widetilde{\xi},\infty}(\phi_1) = \int_{\widetilde{\tau}}^{0} |\phi_1'(\tau)|\,d\tau = \begin{cases} \phi_1(\widetilde{\tau}) & \text{if } \widetilde{\tau} \in [t_2, 0]\,, \\ 2\phi_1(t_2) - \phi_1(\widetilde{\tau}) & \text{if } \widetilde{\tau} \in \left[-\frac{1}{2}, t_2\right]\,. \end{cases} \tag{3.30}$$

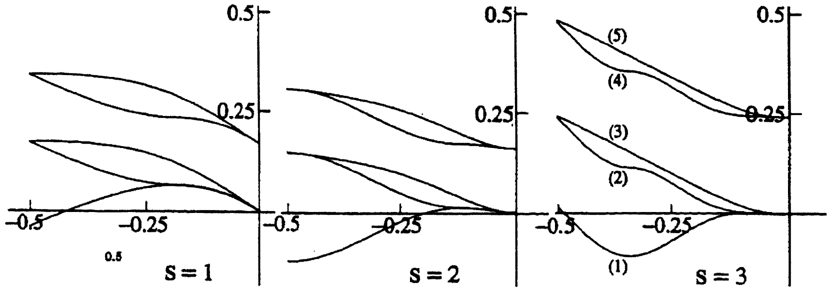

Fig. 3. Graphs of $\phi_s(\widetilde{\tau})$, $s = 1, 2, 3$, $\widetilde{\tau} \in \left[-\frac{1}{2}, 0\right]$, variations and upper bounds; see the text for more details.

The computation of the zeros of $\phi_s'(\widetilde{\tau})$, however, may not be efficient in an algorithm. We can avoid this by constructing for the variations upper bounds as functions of $\widetilde{\tau}$. For example, we found for the first few $\phi_s(\widetilde{\tau})$, the following simple upper bounds for $\widetilde{\tau} \in \left[-\frac{1}{2}, 0\right]$:

$$\begin{aligned} \mathcal{V}_{\widetilde{\xi},\infty}(\phi_1) &\leq \frac{-3\,\widetilde{\tau}}{4(1+4.8\widetilde{\tau}^2)}, \\ \mathcal{V}_{\widetilde{\xi},\infty}(\phi_2) &\leq \frac{105\,\widetilde{\tau}^2}{32(1+18\widetilde{\tau}^2)}, \\ \mathcal{V}_{\widetilde{\xi},\infty}(\phi_3) &\leq \frac{-3465\,\widetilde{\tau}^3}{128(1+52\widetilde{\tau}^2)}. \end{aligned} \tag{3.31}$$

The bounds fit at the origin and are slightly larger at $\widetilde{\tau} = -\frac{1}{2}$.

In Fig. 3 we give the graphs of $\phi_s(\widetilde{\tau})$, $s = 1$ (left), $s = 2$ (middle), and $s = 3$ (right) for $\widetilde{\tau} \in \left[-\frac{1}{2}, 0\right]$. The first graph from the bottom is for $\phi_s(\widetilde{\tau})$, the second one is for the variation in (3.26), and the third one is for the upper bound given in (3.31). The fourth graph is for the variation in (3.29), and the fifth one is the upper bound. The fourth and fifth curves are just equal to the second and third ones shifted upwards because of the variations over $\left[-1, -\frac{1}{2}\right]$, which equal 0.1692, 0.1602, 0.2415, for $s = 1, 2, 3$, respectively. As we explained after (3.29), in (3.29) we consider $\widetilde{\tau} \in \left[-\frac{1}{2}, 0\right]$, and the variations contain contributions from $\left[-1, -\frac{1}{2}\right]$.

3.2. *Negative a*

In this case, we consider the function $U\left(-\frac{1}{2}\mu^2, \mu t\sqrt{2}\right)$. This function satisfies the differential equation

$$\frac{d^2w}{dt^2} = \mu^4(t^2 - 1)w\,. \tag{3.32}$$

For expansions in terms of elementary functions, three intervals should be distinguished: $(-\infty, -1-\delta]$, $[-1+\delta, 1-\delta]$, and $[1+\delta, \infty)$ (the turning points $t = \pm 1$ should be avoided). We only consider the interval $[1+\delta, \infty)$; for the other intervals we refer to [9].

3.2.1. *The case* $t > 1$

We write (see [9, (2.9)])

$$U\left(-\frac{1}{2}\mu^2, \mu t\sqrt{2}\right) = \frac{h(\mu)\, e^{-\mu^2\xi}}{(t^2-1)^{\frac{1}{4}}} F_\mu(t) \tag{3.33}$$

where $h(\mu)$ is defined in (3.13), $F_\mu(t)$ is expanded in the form

$$F_\mu(t) \sim \sum_{s=0}^{\infty} \frac{\phi_s(\tau)}{\mu^{2s}}, \tag{3.34}$$

$$\tau = \frac{1}{2}\left[\frac{t}{\sqrt{t^2-1}} - 1\right], \tag{3.35}$$

$$\xi = \frac{1}{2} t\sqrt{t^2-1} - \frac{1}{2}\ln[t + \sqrt{t^2-1}], \tag{3.36}$$

and the coefficients $\phi_s(\tau)$ are as in (3.12); see also (3.15) and (3.17).

We can derive (3.34) as (3.12) for $a > 0$. The function $F(\tau) = F_\mu(t)$ satisfies the equation (compare this with (3.16))

$$\mu^2 \frac{dF}{d\tau} = -4\frac{d}{d\tau}\left[\tau^2(\tau+1)^2 \frac{dF}{d\tau}\right] - \frac{1}{4}(20\tau^2 + 20\tau + 3)F. \tag{3.37}$$

For the function $V(a, z)$, we have

$$V\left(-\frac{1}{2}\mu^2, \mu t\sqrt{2}\right) = \frac{e^{\mu^2\xi}}{\mu\sqrt{\pi}\, h(\mu)(t^2-1)^{\frac{1}{4}}} P_\mu(t), \quad P_\mu(t) \sim \sum_{s=0}^{\infty}(-1)^s \frac{\phi_s(\tau)}{\mu^{2s}}, \tag{3.38}$$

where the $\phi_s(\tau)$ are the same as in (3.34).

For the derivatives, we have

$$U'\left(-\frac{1}{2}\mu^2, \mu t\sqrt{2}\right) = -\frac{\mu}{\sqrt{2}} h(\mu)(t^2-1)^{\frac{1}{4}} e^{-\mu^2\xi}\, G_\mu(t), \quad G_\mu(t) \sim \sum_{s=0}^{\infty} \frac{\psi_s(\tau)}{\mu^{2s}}, \tag{3.39}$$

and

$$V'\left(-\frac{1}{2}\mu^2, \mu t\sqrt{2}\right) = \frac{(t^2-1)^{\frac{1}{4}} e^{\mu^2\xi}}{\sqrt{2\pi} h(\mu)} Q_\mu(t), \quad Q_\mu(t) \sim \sum_{s=0}^{\infty}(-1)^s \frac{\psi_s(\tau)}{\mu^{2s}}. \tag{3.40}$$

The coefficients ψ_s are the same as in (3.18); see also (3.19) and (3.20).

The functions $F_\mu(t)$, $G_\mu(t)$, $P_\mu(t)$, and $Q_\mu(t)$ introduced in the asymptotic representations satisfy the following exact relation:

$$F_\mu(t)\, Q_\mu(t) + G_\mu(t)\, P_\mu(t) = 2. \tag{3.41}$$

Table 5. Ratios $|R_n(\mu,t)|/R_n^{(e)}(\mu,t)$; $z=2t\sqrt{a}\,, n=3$.

t	1.5	2.0	3.0	5.0	10	20	50
$a=-1$	.29990	.57546	.80676	.93078	.98282	.99572	.99932
$a=-5$	.69226	.86898	.95344	.98522	.99652	.99914	.99986
$a=-10$	.81624	.92930	.97608	.99256	.99826	.99956	.99994
$a=-50$	.95602	.98488	.99510	.99850	.99964	.99992	.99998
$a=-100$	.97744	.99236	.99754	.99924	.99982	.99996	1.0000

3.2.2. *Error bounds of the expansion*

We write the expansion in (3.34) with remainder:

$$F_\mu(t)=\sum_{s=0}^{n-1}\frac{\phi_s(\tau)}{\mu^{2s}}+R_n(\mu,t)\,. \tag{3.42}$$

For the present values of the parameters, the remainder $R_n(\mu,t)$ can be bounded as follows, see [7, p. 366],

$$|R_n(\mu,t)|\le \exp\left[\frac{2\mathcal{V}_{\infty,\xi}(\phi_1)}{|\mu^2|}\right]\frac{\mathcal{V}_{\infty,\xi}(\phi_n)}{|\mu^2|^n}\,. \tag{3.43}$$

In Table 5, we show the ratios $|R_n(\mu,t)|/R_n^{(e)}(\mu,t)$ (with $n=3$) where $R_n^{(e)}(\mu,t)$ is the right-hand side of (3.43).

From the first few $\phi_s(\tau)$ given in (3.17) and the recursion relation in (3.15), it follows that all coefficients in these polynomials have the sign of $(-1)^s$. Hence, for $t>1$, that is, $\tau\ge 0$, the variations in (3.43) can be easily obtained. We have for $n\ge 1$, using (2.9),

$$\mathcal{V}_{\infty,\xi}(\phi_n)=(-1)^n\int_0^\tau \phi_n'(\sigma)\,d\sigma=(-1)^n\phi_n(\tau)=|\phi_n(\tau)|\,. \tag{3.44}$$

4. Obtaining Error Bounds by Using Integrals

A systematic approach for constructing error bounds of remainders in uniform asymptotic expansions is available only for expansions derived from differential equations; see [7]. In this section, we consider a method for expanding (3.11), using an integral representation of the function $U(a,z)$. For this approach, it is convenient to concentrate on large positive values of z and to construct an expansion that holds uniformly with respect to $a\in[0,\infty)$. This expansion reduces to the Poincaré-type expansion in (2.1) when a is fixed after expanding the quantities in the expansion that depend on $\lambda=a/z^2$ for small values of this parameter. In fact, by writing $\mu=z\sqrt{2\lambda}$ and $t=1/(2\sqrt{\lambda})$, the same can be done in the expansion given in (3.11) and (3.12).

4.1. *An integration by parts procedure*

We summarize from [9] and start with the integral representation

$$U(a,z)=\frac{e^{-\frac{1}{4}z^2}}{\Gamma(a+\frac{1}{2})}\int_0^\infty w^a e^{-\frac{1}{2}w^2-zw}\,\frac{dw}{\sqrt{w}},\quad a>-\frac{1}{2},\tag{4.1}$$

which we write in the form

$$U(a,z)=\frac{z^{a+\frac{1}{2}}\,e^{-\frac{1}{4}z^2}}{\Gamma(a+\frac{1}{2})}\int_0^\infty e^{-z^2\phi(w)}\,\frac{dw}{\sqrt{w}}\tag{4.2}$$

where

$$\phi(w)=w+\frac{1}{2}w^2-\lambda\ln w,\quad \lambda=\frac{a}{z^2}=\frac{1}{4t^2}\tag{4.3}$$

where t is used earlier in the notation $U\left(\frac{1}{2}\mu^2,\mu t\sqrt{2}\right)$. The positive saddle point w_0 of $\phi(w)$ is

$$w_0=\frac{1}{2}[\sqrt{1+4\lambda}-1]\,.\tag{4.4}$$

A standard form of (4.2) is obtained by using the transformation

$$\phi(w)=s-\lambda\ln s+A\tag{4.5}$$

where A does not depend on s or w; we prescribe that $w=0$ should correspond with $s=0$ and $w=w_0$ with $s=\lambda$, the saddle point in the s-plane. This gives

$$A=\frac{1}{2}w_0^2+w_0-\lambda\ln w_0-\lambda+\lambda\ln\lambda\,,\tag{4.6}$$

$$U(a,z)=\frac{z^{a+\frac{1}{2}}\,e^{-\frac{1}{4}z^2-Az^2}}{(1+4\lambda)^{\frac{1}{4}}\Gamma(a+\frac{1}{2})}\int_0^\infty s^a e^{-z^2 s}f(s)\,\frac{ds}{\sqrt{s}}\tag{4.7}$$

where

$$f(s)=(1+4\lambda)^{\frac{1}{4}}\sqrt{\frac{s}{w}\,\frac{dw}{ds}}=(1+4\lambda)^{\frac{1}{4}}\sqrt{\frac{w}{s}}\,\frac{s-\lambda}{w^2+w-\lambda}\,.\tag{4.8}$$

By normalizing with the quantity $(1+4\lambda)^{\frac{1}{4}}$, we obtain $f(\lambda)=1$, as can be verified from (4.8) and a limiting process (using l'Hôpital's rule).

For $\lambda\to 0$, the saddle point w_0 tends to zero, and the mapping becomes

$$\frac{1}{2}w^2+w=s\,.\tag{4.9}$$

It is not difficult to verify that for $\lambda=0$, we have

$$f(s)=\sqrt{\frac{1+\sqrt{1+2s}}{2(1+2s)}}\,.\tag{4.10}$$

If $\lambda \neq 0$, the transformation (4.5) also can be written in the form

$$\lambda w = w_0\, s\, e^{\frac{1}{\lambda}\left(\frac{1}{2}w^2+w-s-\frac{1}{2}w_0^2-w_0+\lambda\right)}, \tag{4.11}$$

in which form no logarithms occur.

We introduce a sequence of functions $\{f_k\}$ with $f_0(s) = f(s)$ and

$$f_{k+1}(s) = \sqrt{s}\,\frac{d}{ds}\left[\sqrt{s}\,\frac{f_k(s) - f_k(\lambda)}{s-\lambda}\right], \quad k = 0, 1, 2, \ldots. \tag{4.12}$$

The expansion in (3.12) can be obtained by using an integration by parts procedure. Consider the integral

$$F_a(z) = \frac{1}{\Gamma(a+\frac{1}{2})}\int_0^\infty s^a e^{-z^2 s} f(s)\,\frac{ds}{\sqrt{s}}. \tag{4.13}$$

We have (with $\lambda = a/z^2$)

$$\begin{aligned} F_a(z) &= z^{-2a-1} f(\lambda) + \frac{1}{\Gamma(a+\frac{1}{2})}\int_0^\infty s^a e^{-z^2 s}[f(s) - f(\lambda)]\,\frac{ds}{\sqrt{s}} \\ &= z^{-2a-1} f(\lambda) - \frac{1}{z^2\Gamma(a+\frac{1}{2})}\int_0^\infty \sqrt{s}\,\frac{f(s)-f(\lambda)}{s-\lambda}\, de^{-z^2(s-\lambda\ln s)} \\ &= z^{-2a-1} f(\lambda) + \frac{1}{z^2\Gamma(a+\frac{1}{2})}\int_0^\infty s^a e^{-z^2 s} f_1(s)\,\frac{ds}{\sqrt{s}} \end{aligned}$$

where f_1 is given (4.12) with $f_0 = f$. Repeating this procedure we obtain

$$U(a,z) \sim \frac{e^{-\frac{1}{4}z^2 - Az^2}}{z^{a+\frac{1}{2}}\,(1+4\lambda)^{\frac{1}{4}}}\sum_{k=0}^\infty \frac{f_k(\lambda)}{z^{2k}}. \tag{4.14}$$

The factor in front of the series in (4.14) and the factor in (3.11) are the same. This can be verified by using $a = \frac{1}{2}\mu^2$ and $z = \mu\sqrt{2}t$. Also, the two series correspond termwise with each other, the relation between the coefficients being

$$\phi_k(\widetilde{\tau}) = \frac{(-1)^k}{(2t^2)^k} f_k(\lambda), \quad \widetilde{\tau} = \frac{1}{2}\left[\frac{1}{\sqrt{4\lambda+1}} - 1\right]. \tag{4.15}$$

For example, we have

$$f_0(\lambda) = 1, \quad f_1(\lambda) = -\frac{(2\widetilde{\tau}+1)^2}{24(\widetilde{\tau}+1)}(20\widetilde{\tau}^2 + 30\widetilde{\tau} + 9). \tag{4.16}$$

We write (4.14) with a remainder:

$$U(a,z) = \frac{e^{-\frac{1}{4}z^2 - Az^2}}{z^{a+\frac{1}{2}}\,(1+4\lambda)^{\frac{1}{4}}}\left[\sum_{k=0}^{n-1} \frac{f_k(\lambda)}{z^{2k}} + \frac{1}{z^{2n}} R_n(a,z)\right] \tag{4.17}$$

where

$$R_n(a,z) = \frac{z^{2a+1}}{\Gamma(a+\frac{1}{2})}\int_0^\infty s^a e^{-z^2 s} f_n(s)\,\frac{ds}{\sqrt{s}}. \tag{4.18}$$

4.2. *Bounding the remainder*

From (4.5) and (4.8), we infer that $f(s) = \mathcal{O}(s^{-1/4})$ as $s \to \infty$ (see also (4.10) for a simple verification when $\lambda = 0$). So, $f(s)$ is bounded on $[0, \infty)$. We also can prove (which will not be done here) from (4.12) that $f_n(s) = \mathcal{O}(s^{-1/4})$, $n \geq 1$. Hence, the functions $f_n(s)$ can be bounded by $|f_n(s)| \leq M_n(\lambda)$ for $s \geq 0$. When using this bound in (4.18), we indeed obtain an upper bound for $|R_n(a, z)|$, but this bound may not be realistic.

A much better bound is obtainable by estimating $|f_n(s)|$ accurately near the point $s = \lambda$ (where the integrand of (4.18) has its peak) and accepting a rough estimate for other s-values. This can be achieved by using a "weight function" $w_n(s, \lambda)$ and by writing

$$|f_n(s)| \leq [|f_n(\lambda)| + M_n(\lambda)]\, w_n(s, \lambda)\,, \tag{4.19}$$

where, for example, we take

$$w_n(s, \lambda) = [(s/\lambda)^{-\lambda} e^{s-\lambda}]^{\sigma_n}\,. \tag{4.20}$$

We have $w_n(\lambda, \lambda) = 1$. Observe that for $s = \lambda$, the dominant part $s^a e^{-z^2 s}$ of the integrand in (4.18) assumes its maximal value when a and z are large. We try to find $M_n(\lambda) > 0$ and $\sigma_n \geq 0$ such that (4.19) holds for all $s \geq 0$. Then we obtain the bound

$$|R_n(a, z)| \leq [|f_n(\lambda)| + M_n(\lambda)]\, S_n(a, z) \tag{4.21}$$

where

$$S_n(a, z) = a^{\lambda\sigma_n} e^{-\lambda\sigma_n} \left(1 - \frac{\sigma_n}{z^2}\right)^{\lambda\sigma_n - a - \frac{1}{2}} \frac{\Gamma(a + \frac{1}{2} - \lambda\sigma_n)}{\Gamma(a + \frac{1}{2})}\,. \tag{4.22}$$

For $S_n(a, z)$, we need the conditions

$$z^2 > \sigma_n, \quad a + \frac{1}{2} > \lambda\sigma_n\,. \tag{4.23}$$

The quantity $S_n(a, z)$ is close to unity when $a + z$ is large; because f_n is bounded, the value of σ_n will be small. Numerical calculations show that for $\sigma_n = 1$ and $z \geq 3$, $a \geq 1$, the maximal value of $S_n(a, z)$ is smaller than 1.062.

In Fig. 4, we show the graph of $[(1 + 5\lambda)|f_n(\lambda)| + M_n(\lambda)]$ (the factor $(1 + 5\lambda)$ is chosen for scaling) when we take $\sigma_1 = 1$ in (4.19). We have $M_1(0) = 0$, $f_1(0) = -3/8$, and $f_1(\lambda) \sim 1/(48\lambda)$ for large λ. We also draw the graph of

$$\rho_1(\lambda) = \frac{|R_1(a, z)|}{[|f_1(\lambda)| + M_1(\lambda)] S_1(a, z)}\,, \tag{4.24}$$

the ratio of the exact error and the estimated error. We see a sharp dip at $\lambda = 8.3176\ldots$, which is a zero of $f_1(\lambda)$; for this value of λ, the asymptotic approximation improves, as expected. For large λ, the quantity ρ_1 tends to 1.

We computed $M_1(\lambda)$ in (4.24) as the infimum of $|f_1(s)/w_1(s, \lambda)|$, $s \geq 0$, and this gives a continuous function $M_1(\lambda)$, but it may not be smooth. For example,

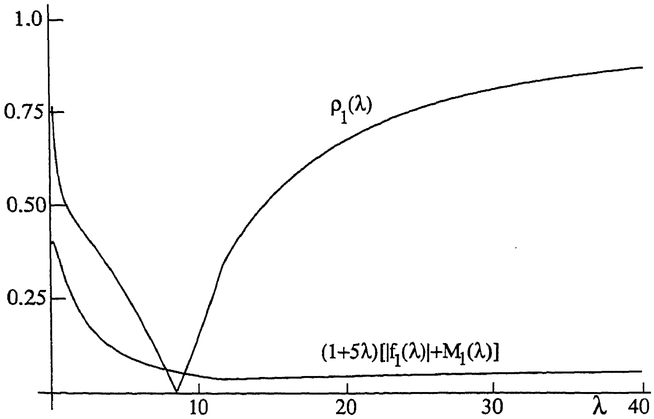

Fig. 4. The graph of $(1+5\lambda)[|f_1(\lambda)| + M_1(\lambda)]$ with $M_1(\lambda)$ introduced in (4.19) (with $\sigma_1 = 1$), and $\rho_1(\lambda)$ from (4.24).

there is a noticeable non-smooth behavior near $\lambda = 11$ because $\inf |f_1(s)/w_1(s,\lambda)|$ occurs for $\lambda < 11$ in a different s-domain than for $\lambda > 11$.

4.3. *Bounding the remainder by using Cauchy-type integrals*

Computing the functions $f_n(s)$ by using formula (4.12) is quite difficult, even when we use computer algebra. The representations contain derivatives and removable singularities (poles) at $s = \lambda$. In particular, these removable poles are very inconvenient when computing the functions $f_n(s)$ near $s = \lambda$.

It is possible, however, to represent $f_n(s)$ as a Cauchy-type integral. The mapping in (4.5) is singular at $w = w_- = -1 - w_0$, the negative saddle point of $\phi(w)$ defined in (4.3). The corresponding value $s_- = s(w_-)$ is located in the half-plane $\Re s < 0$. If $\lambda = 0$, then $w_- = -1$ and the corresponding s-value is $s_- = -\frac{1}{2}$. Refer to (4.10), where indeed $f(s)$ shows a singularity at this point. For large values of λ, we have the estimate (see [9, (4.45)])

$$s_- = s(w_-) \sim -\lambda \left[0.2785 + \frac{0.4356}{\sqrt{\lambda}}\right]. \tag{4.25}$$

For constructing the Cauchy-type integrals, we use the property that the functions $f_n(s)$ are analytic functions in a domain $\mathcal{D}$ in the half-plane $\Re s_-$; in particular, $\mathcal{D}$ contains a neighborhood of the positive real axis.

As in [4], we start from

$$f_n(s) = \frac{1}{2\pi i}\int_{\mathcal{C}} Q_0(\sigma,\lambda,s) f_n(\sigma)\, d\sigma, \quad Q_0(\sigma,\lambda,s) = \frac{1}{\sigma - s}, \tag{4.26}$$

where $s \in \mathcal{D}$ and $\mathcal{C}$ is a contour in $\mathcal{D}$ around the point $\sigma = s$. Using the recursion (4.12), and integrating by parts, we obtain

$$f_n(s) = \frac{1}{2\pi i}\int_{\mathcal{C}} Q_1(\sigma,\lambda,s) f_{n-1}(\sigma) d\sigma \tag{4.27}$$

where $\mathcal{C}$ is a contour in $\mathcal{D}$ around the points $\sigma = \lambda$ and $\sigma = s$, and

$$Q_1(\sigma, \lambda, s) = -\frac{1}{2(\sigma - \lambda)}\left[Q_0 + 2\sigma\frac{\partial}{\partial\sigma}Q_0\right] = \frac{\sigma + s}{2(\sigma - \lambda)(\sigma - s)^2}\,. \tag{4.28}$$

Continuing this, we obtain for $n = 0, 1, 2, \ldots,$

$$f_n(s) = \frac{1}{2\pi i}\int_{\mathcal{C}} Q_n(\sigma, \lambda, s) f(\sigma)\, d\sigma\,. \tag{4.29}$$

The rational functions Q_n follow from the recursion relation

$$Q_n = -\frac{1}{2(\sigma - \lambda)}\left[Q_{n-1} + 2\sigma\frac{\partial}{\partial\sigma}Q_{n-1}\right]. \tag{4.30}$$

For example, we have

$$Q_2(\sigma, \lambda, s) = \frac{3\sigma^3 - \lambda\sigma^2 - \sigma s^2 - \lambda s^2 + 6\sigma^2 s - 6\lambda\sigma s}{4(\sigma - \lambda)^3(\sigma - s)^3}\,. \tag{4.31}$$

The coefficients $f_k(\lambda)$ in (4.14) follow from (4.29) by substituting $s = \lambda$.

We can obtain a bound for $f_n(s)$ by using the representation in (4.29) and by selecting a special contour. We take for $\mathcal{C}$ the vertical line $\Re\sigma = -\sigma_0$ where $\sigma_0 > 0$. First we write the quantities Q_n in a special form:

$$Q_1(\sigma, \lambda, s) = \frac{2\lambda - p + 2q}{2\,p^2\,q} = \frac{\lambda}{p^2 q} - \frac{1}{2pq} + \frac{1}{p^2} \tag{4.32}$$

where

$$p = \sigma - s, \quad q = \sigma - \lambda\,. \tag{4.33}$$

Similarly,

$$Q_2(\sigma, \lambda, s) = \frac{8\lambda^2 q + 16\lambda q^2 + 8q^3 + 4p\lambda^2 - 4pq^2 - 2\lambda p^2 - p^2 q}{4\,p^3\,q^3}\,, \tag{4.34}$$

which also can be written as a sum of partial fractions in which σ occurs only in the denominator.

For $\sigma \in \mathcal{C}$, we write $\sigma = -\sigma_0 + i\tau$, $\tau \in \mathbb{R}$. For $s \geq 0$ and $\lambda \geq 0$, we have

$$|p| \geq |\sigma| = \sqrt{\sigma_0^2 + \tau^2}, \quad |q| \geq |\lambda + \sigma_0 + i\tau| \geq \sqrt{\sigma_0^2 + \tau^2}\,. \tag{4.35}$$

This gives for Q_1 the bound

$$|Q_1(\sigma, \lambda, s)| \leq \frac{\lambda}{(\sigma_0^2 + \tau^2)^{3/2}} + \frac{3}{2(\sigma_0^2 + \tau^2)}\,. \tag{4.36}$$

We also need a bound of $f(s)$ for $s \in \mathcal{C}$ (we know that this function is bounded on $\mathcal{C}$, see beginning of Sec. 4.2). Let

$$M(\sigma_0, \lambda) = \max_{s \in \mathcal{C}} |f(s)|\,. \tag{4.37}$$

This gives for the remainder defined in (4.18) the upper bound

$$|R_1(a,z)| \le M(\sigma_0, \lambda)\, \frac{4\lambda + 3\pi\sigma_0}{4\pi\sigma_0^2}\,. \tag{4.38}$$

Similarly,

$$|Q_2(\sigma, \lambda, s)| \le \frac{3\lambda^2}{2(\sigma_0^2+\tau^2)^{5/2}} + \frac{11\lambda}{4(\sigma_0^2+\tau^2)^2} + \frac{13}{8(\sigma_0^2+\tau^2)^{3/2}}\,, \tag{4.39}$$

$$|R_2(a,z)| \le M(\sigma_0, \lambda)\, \frac{9\lambda^2 + 11\pi\lambda\sigma_0 + 26\sigma_0^2}{16\pi\sigma_0^4}\,, \tag{4.40}$$

$$|Q_3(\sigma, \lambda, s)| \le \frac{15\lambda^3}{(\sigma_0^2+\tau^2)^{7/2}} + \frac{61\lambda^2}{2(\sigma_0^2+\tau^2)^3} + \frac{43\lambda}{2(\sigma_0^2+\tau^2)^{5/2}} + \frac{81}{8(\sigma_0^2+\tau^2)^2}\,, \tag{4.41}$$

$$|R_3(a,z)| \le M(\sigma_0, \lambda)\, \frac{768\lambda^3 + 549\pi\lambda^2\sigma_0 + 1376\lambda\sigma_0^2 + 243\pi\sigma_0^3}{96\pi\sigma_0^6}\,. \tag{4.42}$$

The singularity s_-, estimated in (4.25), is of order $\mathcal{O}(\lambda)$, and it follows that σ_0 also can be taken to be of order $\mathcal{O}(\lambda)$. When we choose σ_0 in this way, we see that the first three quantities Q_n, for this choice of $\mathcal{C}$, are of order $\mathcal{O}(1/\lambda^{n+1})$ as $\lambda \to \infty$, and the remainders are of order $\mathcal{O}(1/\lambda^n)$. For higher values of n we see a similar behavior.

We conclude that the estimates of the Q_n can be obtained quite easily, and that only the estimate of $|f(s)|$ is needed for obtaining bounds of $R_n(z,a)$. From numerical verifications, we infer that (on $\mathcal{C}$) $|f(s)|$ is maximal at $s = -\sigma_0$. Hence, we can take $M(\sigma_0, \lambda) = |f(-\sigma_0)|$.

Comparing the numerical bounds with those obtained by the method of Sec. 3.2.2, we conclude that the present bounds are less realistic unless λ is very large.

5. Numerical Aspects

For the computation of the numerical upper bounds of the remainders in the expansion, we used computer algebra for manipulating the formulas. This already became quite complicated, even though we did not consider complex parameters. The evaluation of the variations of the coefficients ϕ_n in the uniform expansions can be done by computing the zeros of the derivatives of ϕ_n. When using computer algebra this is an easy job because the ϕ_n are polynomials. For a fast algorithm, say in Fortran, one may use precomputed values of these zeros and corresponding values of ϕ_n in order to avoid the time consuming computation of the zeros.

For computing values of the remainders used in the Tables 3–5, we needed accurate values of the asymptotic expansions and the function $U(a,x)$ because of the subtraction of two quantities with many corresponding leading digits.

For example, for computing $\widetilde{R}_n(\mu,t)$ of (3.24) for $n=3$, $a=100$, and $t=50$ (which corresponds with $x=1000$), the values of $\widetilde{F}_\mu(t)$ and the asymptotic series in (3.24) (with $n=3$) are

$$0.99999\ 96252\ 38198\ 34461, \quad 0.99999\ 96252\ 38198\ 34799,$$

respectively, with 17 corresponding digits. We have computed these values with 30 digits accuracy (using Maple 7) and developed new algorithms with adjustable precision, based on quadrature methods.

It was necessary to develop new algorithms for the parabolic cylinder functions for large values of the parameters because when we used the Maple 7 Library function *CylinderU*(a,x) or the relation with the Whittaker function in (2.6), the answers were not reliable, and the computing time was increasing considerably, when the parameters are large.

For example, the evaluation of $U(10,100)$ with Digits $=50$ took about 100 seconds and gave an answer of order 10^{832}, whereas the answer should be exponentially small. When we use our code with Digits $=30$, we obtain within a few seconds the answer $0.182463637678584422244199909618045 \times 10^{-1106}$ which has 27 correct leading digits. We will present these real parameter Maple codes for the numerical evaluation of $U(a,x)$ and $V(a,x)$, and their derivatives, on the web site of our project `http://turing.wins.uva.nl/thk/specfun/compalg.html`. Fortran versions of these codes will be developed in a following project.

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