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A Numerical Algorithm for the Evaluation of Weber Parabolic Cylinder Functions $U(a,x)$, $V(a,x)$, and $W(a, \pm x)$*

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Weber's parabolic cylinder functions $U(a,x)$, $V(a,x)$, and $W(a, \pm x)$ have recently found wide applications as approximations to quantum mechanical and semi-classical wavefunctions propagating through potential wells or barriers. Available algorithms for their numerical evaluation are inapplicable in some ranges of the two arguments. In this paper we present a new algorithm, based on the combined use of F. W. J. Olver's (*J. Res. Nat. Bur. Stand. Sect. B* **63** (1959), 131) uniform asymptotic expansions and E. T. Whittaker's (*Proc. London Math. Soc.* **35** (1903), 417) complex recurrence relations, to extend their range of usefulness. Using double precision arithmetic, the algorithm generates greater than single precision values of the functions and their derivatives on a Univac 1182.

1. INTRODUCTION

As approximations to wavefunctions in quantum mechanical calculations, Weber's parabolic cylinder functions have received considerable attention. They are used in WKBJ-type problems involving two or more transition or turning points [2, 5, 6, 11, 12, 15, 20, 22, 26–29]. They have also recently been employed in a quantum rate theory to describe proton transfer reactions in double well potentials [31]. Our

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interest in the evaluation of these functions grew out of our work on piecewise analytical solutions for the Schroedinger equation [9, 10, 16] whereby we approximate the potential locally by a polynomial function. We then use the continuity conditions to form the complete wavefunction as a composite of the local wavefunctions. Previously, we had been able to use only piecewise linear polynomial approximations, giving rise to a basis of Airy functions. A more accurate approximation to the potential can be formed by a quadratic polynomial. The resulting wavefunction is a solution of Weber's complex linear second-order differential equation [30],

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

$D_\nu(z)$ is Whittaker's notation for parabolic cylinder functions, and its value is determined upon specifying a point in the two dimensional complex space (z, ν). $D_\nu(z)$ is an entire function of both variables. Throughout the next ν and z will denote complex variables while their real counterparts will be denoted a, a real parameter, and x a real independent variable. It is clear that for special values of the variables (x, a), (1.1) can be transformed into either the equation for the generalized harmonic oscillator functions, which we write as $U(a, x)$ and $V(a, x)$, or the equation for propagation through a potential barrier, with a set of solutions $W(a, \pm x)$.

To allow the greatest flexibility on using (1.1) or specifically its two distinct real forms as approximations to more complicated differential equations, we must be able to evaluate these functions for arbitrary values of ν and z (a and x). The number of numerical studies on the Weber functions is voluminous [1, 8, 13, 14, 18, 21–25, 28]. While there exist asymptotic formulas for large magnitudes of the parameter ν and/or the spatial variable z, and power series for small magnitudes of ν and z, there are still ranges for which, heretofore, no accurate or convenient means of evaluation existed. Extrapolation from a table of values [8, 18] is both inefficient and inconvenient. Employing an algorithm developed by Gordon, integral representations for the $U(a, x)$ and $V(a, x)$ have been evaluated by Gaussian quadrature for small values of the parameter a $(-1.5 < a < 1.8)$ and large values of x [14, 28]. In the case of $U(a, x)$, attempts to extend the range of a by direct forward recurrence lead, as to be expected (see Section 3), to a loss of accuracy.

A recent thorough analysis of the asymptotic behaviour ($|\nu|$ large) of the parabolic cylinder functions, and in particular $U(a, x)$, $V(a, x)$, $W(a, \pm x)$, is in a series of papers by Olver [21–23]. While his asymptotic representations are valid only for large $|\nu|$, they have the advantage of being uniform in the spatial variable z. Consequently we were left only with the problem of devising a convenient method to evaluate these functions and their derivatives when the parameters are in the moderate range.

In this paper we present an algorithm for the computation of the parabolic cylinder functions $U(a, x)$, $V(a, x)$, $W(a, \pm x)$ and their derivatives for arbitrary values of the variables. Those regions of the (x, a) plane, previously inaccessible by accurate and efficient computational techniques, are covered by a set of complex recurrence relations first derived by Whittaker. For large $|a|$, the uniform asymptotic formulas of Olver are employed directly, and for moderate $|a|$ they are employed to generate starting values for the recurrence relations at some large initial indices. The recurrence relations are then used directly, either forwards or backwards, to evaluate the functions at the desired moderate values of a. In Section 2 we define our choice of standard functions for the algorithms. In Section 3 we examine the recurrence relations and specify the special discrete paths of the complex recurrence index. We outline the numerical evaluation of $U(a, x)$ and $V(a, x)$ in Section 4 and that of $W(a, \pm x)$ in Section 5.

2. Choice of Standard Functions

For most physical problems only the two real standard forms of (1.1) are of importance. The first, obtained by setting $\nu + \frac{1}{2} = -a$ and $z = x$, is the generalized harmonic oscillator equation

$$\frac{d^2 D_{-a-1/2}(x)}{dx^2} - \left(\frac{1}{4}x^2 + a\right) D_{-a-1/2}(x) = 0. \tag{2.1}$$

For standard solutions we take as the two linearly independent solutions $U(a, x)$ and $V(a, x)$ as defined by Miller [17, 18]

$$U(a, x) = D_{-a-1/2}(x), \tag{2.2}$$

$$V(a, x) = (1/\pi)\,\Gamma(\tfrac{1}{2} + a)\{D_{-a-1/2}(x) \sin a\pi + D_{-a-1/2}(-x)\}. \tag{2.3}$$

When $a + \frac{1}{2}$ is zero or a negative integer, $U(a, x)$ can be related to the Hermite polynomials

$$U(-n - \tfrac{1}{2}, x) = 2^{-n/2} e^{-x^2/4} H_n(x/\sqrt{2}). \tag{2.4}$$

For a negative $U(a, x)$ and $V(a, x)$ are oscillating functions between the turning points $x_{TP} = \pm 2\sqrt{-a}$ (see Fig. 1a), and as pointed out by Miller [18] and Olver [21] one could replace $V(a, x)$ by the companion solution $\bar{U}(a, x)$ of equal modulus

$$\bar{U}(a, x) = \Gamma(\tfrac{1}{2} - a)\, V(a, x) = U(a, x) \tan \pi a + U(a, -x) \sec \pi a. \tag{2.5}$$

When $a + \frac{1}{2}$ is not zero or a negative integer, $U(a, \pm x)$ are an alternate pair of solutions. In particular for a positive, $U(a, x)$ and $U(a, -x)$ are exponentially decreasing and increasing functions, respectively.

The second standard form, obtained by setting $\nu + \frac{1}{2} = -ia$ and $z = xe^{-\pi i/4}$ describes the propagation through or over a parabolic potential barrier

$$\frac{d^2 D_{-ia-1/2}(xe^{-\pi i/4})}{dx^2} + \left(\frac{1}{4}x^2 - a\right) D_{-ia-1/2}(xe^{-\pi i/4}) = 0. \tag{2.6}$$

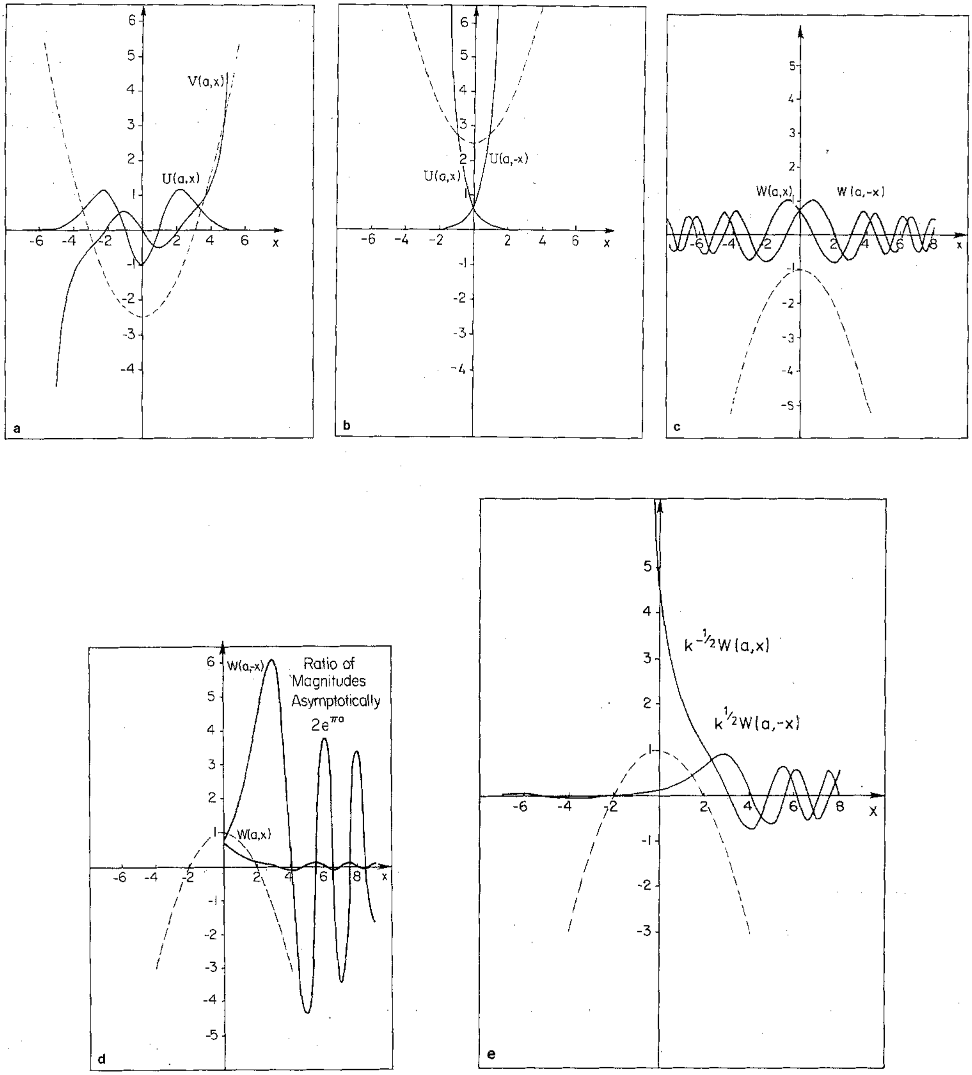

FIG. 1. (a) $U(a, x)$ and $V(a, x)$ for $a = -2.5$ and (b) $U(a, x)$ and $U(a, -x)$ for $a = 2.5$. Coefficient function $(\frac{1}{4}x^2 + a)$ is indicated by broken lines. $W(a, x)$ and $W(a, -x)$ for (c) $a = -1$ and (d) $a = 1$. Coefficient function $(a - \frac{1}{4}x^2)$ is indicated by broken lines. (e) Components of complex function $E(a, x)$ for $a \doteq 1$.

In terms of Miller's notation we have

$$U(ia, xe^{-\pi i/4}) = D_{-ia-1/2}(xe^{-\pi i/4}). \tag{2.7}$$

Two real solutions to (2.6), $W(a, \pm x)$, can be defined in terms of a complex function $E(a, x)$, which with its complex conjugate forms another pair of linearly independent solutions:

$$E(a,x)=\sqrt{2}e^{\pi a/4+(i/2)(\pi/4+\phi)}D_{-ia-1/2}(xe^{-\pi i/4}), \qquad x\geqslant 0, \tag{2.8}$$

$$=k^{-1/2}W(a,x)+ik^{1/2}W(a,-x), \tag{2.9}$$

where $\phi=\arg\Gamma(\frac{1}{2}+ia)$ and $k=\sqrt{1+e^{2\pi a}}-e^{\pi a}$. The value of ϕ is not necessarily in the principal range $(-\pi,\pi]$, but rather it is defined by continuity with $\phi=0$ when $a=0$ and $\phi=a\ln a-a+O(a^{-1})$ as $a\to+\infty$.

For a few convenient values of the parameters a, we have plotted in Fig. 1 the functions $U(a,\pm x)$, $V(a,x)$, $W(a,\pm x)$, and the components of $E(a,x)$ with respect to the x variable. We make reference to these graphs in order to emphasize the characteristic behaviour and disparate nature of the standard functions. To describe the propagation through a potential barrier, the set of functions most closely satisfying Miller's criteria are $k^{-1/2}W(a,x)$ and $k^{+1/2}W(a,-x)$.

3. Recurrence Relations

The recurrence formulas for the parabolic cylinder function $D_\nu(z)$,

$$D_{\nu+1}(z)-zD_\nu(z)+\nu D_{\nu-1}(z)=0, \tag{3.1}$$

$$D'_\nu(z)+(z/2)D_\nu(z)-\nu D_{\nu-1}(z)=0, \tag{3.2}$$

$$D'_\nu(z)-(z/2)D_\nu(z)+D_{\nu+1}(z)=0, \tag{3.3}$$

were derived by Whittaker [32] from the contour integral representation

$$D_\nu(z)=-\frac{\Gamma(\nu+1)}{2\pi i}e^{-(1/4)z^2}\int_\infty^{0+}e^{-zt-(1/2)t^2}(-t)^{-\nu-1}\,dt$$

$$-\pi<\arg(-t)<\pi, \qquad \mathrm{Re}(\nu)<0. \tag{3.4}$$

Integration of Eq. (3.4) by parts yields (3.1). Differentiating formally under the integral we obtain (3.2). We solve for $D_{\nu-1}(z)$ from Eq. (3.1) and substitute the expression into (3.2) to obtain the last relation (3.3). Unless otherwise stated, the prime notation will denote differentiation with respect to the independent variable x or z, which is indicated in the argument of the function. These relations are valid for all complex values of ν and z.

When both variables are real, two sets of relations can be derived from Eqs. (3.1)–(3.3). In terms of the real valued functions $U(a,x)$ and $V(a,x)$ the recursion formulas are as follows:

$$U(a-1,x)-xU(a,x)-(a+\tfrac{1}{2})\,U(a+1,x)=0, \tag{3.5}$$

$$U'(a,x)+\tfrac{1}{2}xU(a,x)+(a+\tfrac{1}{2})\,U(a+1,x)=0, \tag{3.6}$$

$$U'(a,x)-\tfrac{1}{2}xU(a,x)+U(a-1,x)=0, \tag{3.7}$$

and

$$V(a+1,x) - xV(a,x) - (a-\tfrac{1}{2})\,V(a-1,x) = 0, \tag{3.8}$$

$$V'(a,x) - \tfrac{1}{2}xV(a,x) - (a-\tfrac{1}{2})\,V(a-1,x) = 0, \tag{3.9}$$

$$V'(a,x) + \tfrac{1}{2}xV(a,x) - V(a+1,x) = 0. \tag{3.10}$$

For moderate values of a, we want to use these recurrence relations to extend the range of usefulness of Olver's [21] asymptotic expansions. In this paper, only direct recurrence, forwards or backwards, of relations (3.5) and (3.8) with $x \geqslant 0$ is considered. As we will explain in Section 4, the derivatives are used only at the beginning and end of the recurrence process. The stable direction in which to use these recurrence relations directly is suggested from a graph of $U(a,x)$, $V(a,x)$ vs a for constant values x, as in Fig. 2, or by an analysis of the asymptotic form of (3.5) and (3.8). To provide a balance among the terms in the relations, the following inequalities must hold:

$$\left.\begin{array}{l} |U(a-1,x)| > |U(a+1,x)| \\ |V(a+1,x)| > |V(a-1,x)| \end{array}\right. \quad \text{as} \quad a \to +\infty, \ x > 0.$$

For a positive, $U(a,x)$ decays exponentially, and $V(a,x)$ grows exponentially. For a negative, they are oscillatory functions whose moduli are either strictly increasing or decreasing functions of a. Since direct recurrence is generally stable in the direction of increasing function values, relation (3.5) should be started at some large positive index a_+ and recurred backwards (decreasing a) to evaluate $U(a,x)$. Similarly, relation (3.8) should be started at some large negative index a_- and recurred forwards (increasing a) to evaluate $V(a,x)$ (see Fig. 3).

Being second-order homogeneous linear difference equations, relations (3.5) and (3.8) have two independent solutions. To make the above arguments conclusive, it is necessary to show in the case of (3.5), for example, that $U(a,x)$ decreases at least as fast as any other linearly independent solution. Otherwise contributions from the

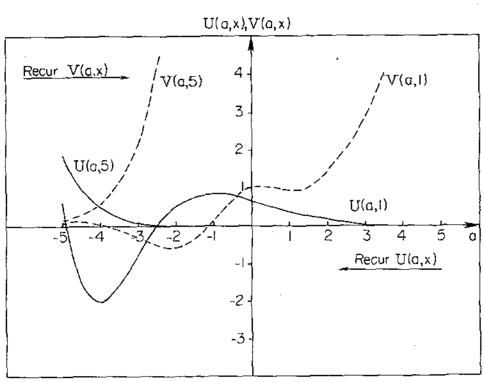

FIG. 2. $U(a,x)$ and $V(a,x)$ as a function of a for fixed values of x.

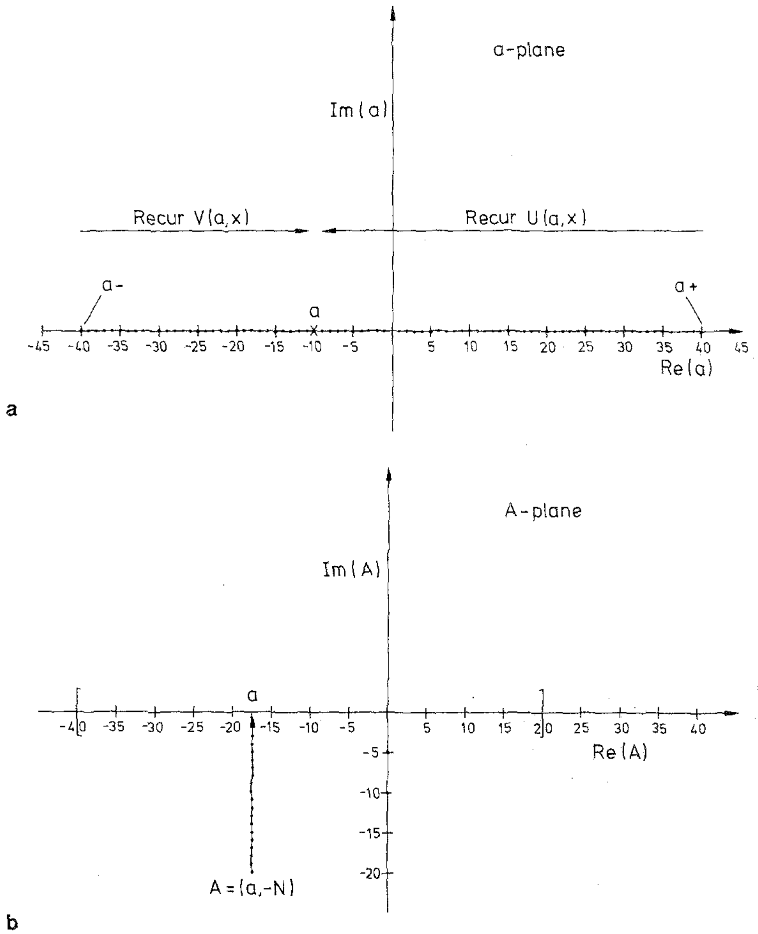

FIG. 3. Typical paths for recurrence index in evaluation of (a) $U(a, x)$ and $V(a, x)$ for $a_- < a < a_+$ and (b) $U(iA, xe^{-\pi i/4})$, where $A = a - iN$ for $-40 < a < 20$.

unwanted solution, introduced by rounding errors, can accumulate and destroy the accuracy. An independent solution of (3.5) is Miller's function $\bar{U}(a, x)$ given in (2.5). Upon comparing the asymptotic forms of $U(a, x)$ and $\bar{U}(a, x)$ for large positive a and fixed $x > 0$ [1], one sees that their ratio decay resembles

$$\lim_{a \to +\infty} \frac{|U(a, x)|}{|\bar{U}(a, x)|} \simeq \cos \pi a e^{-2\sqrt{a}x - O(x^3/\sqrt{a})}.$$

As Miller explained in [1], by recurring Eq. (3.5) backwards from $a_+ \gg a$, the contribution from the dominant solution (with respect to increasing a) is kept negligible. In the case of (3.8) another independent solution is Miller's function $\bar{V}(a, x)$ [18], where

$$\bar{V}(a, x) = \frac{U(a, x)}{\Gamma(\frac{1}{2} - a)}.$$

For a large and negative and fixed $x > 0$, $V(a, x)$ and $\bar{V}(a, x)$ are decreasing oscillating functions with equal modulus and a phase difference of $\pi/2$. The ratio of the two functions is approximated asymptotically by

$$\lim_{a \to -\infty} \frac{V(a, x)}{\bar{V}(a, x)} \simeq \frac{Bi[-((3\,|a|/4)\pi)^{2/3}]}{Ai[-((3\,|a|/4)\pi)^{2/3}]} \sim \frac{\cos((|a|/2)\pi + \pi/4)}{\sin((|a|/2)\pi + \pi/4)},$$

where Bi and Ai are Airy functions. Contributions from the unwanted solution $\bar{V}(a, x)$ introduced by rounding errors wll be random-like, and their effect will be negligible.

We need not restrict ourselves to direct recurrence only of (3.5) and (3.8). As has been pointed out by Miller [19] and Cash and Miller [4] there are many methods involving iteration to compute any well-defined solution of a three-term linear recurrence relation. However, since Olver's asymptotic expansions afford us a simple means to generate the starting values at $a_\pm$ for arbitrary values of x so that direct recurrence could be used in the stable directions, we did not pursue this avenue of solution.

Unfortunately, no analogous set of real recurrence relations is known to exist for either set of independent solutions $k^{\mp 1/2} W(a, \pm x)$ or $E(a, x)$, $E^*(a, x)$. However, we observed that since the recurrence relations are valid for complex values of ν and z, Eqs. (3.1)–(3.3) could be used to recur on $D_{-iA-1/2}(xe^{-\pi i/4})$, where A is a complex parameter, $A = a \pm iN$, $N = 0, 1, \ldots, N_{\max}$. The raising and lowering of the index is now in unit intervals along a line parallel to the imaginary axis in the A-plane (see Fig. 3). Upon recurring to the real axis, i.e., $A = a$, Eqs. (2.5) and (2.6) are used to construct $E(a, x)$ and consequently $k^{\mp 1/2} W(a, \pm x)$. For convenience let us use Miller's notation to express the recurrence relations in terms of the complex function

$$U(iA, z) = D_{-iA-1/2}(z). \tag{3.11}$$

With this substitution, Eqs. (3.1)–(3.3) now have the form

$$U(i(A + i), z) - zU(iA, z) - (iA + \tfrac{1}{2})\, U(i(A - i), z) = 0, \tag{3.12}$$

$$U'(iA, z) + (z/2)\, U(iA, z) + (iA + \tfrac{1}{2})\, U(i(A - i), z) = 0, \tag{3.13}$$

$$U'(iA, z) - (z/2)\, U(iA, z) + U(i(A + i), z) = 0. \tag{3.14}$$

The asymptotic form of $U(iA, xe^{-\pi i/4})$ for $|A| \to \infty$, $|\arg(iA + \frac{1}{2})| \leqslant \pi/2$ and fixed x, $0 \leqslant x < \infty$, is [7]

$$U(iA, xe^{-\pi i/4}) \sim 2^{-1/2} \exp[\tfrac{1}{2}(-iA - \tfrac{1}{2}) \ln(iA + \tfrac{1}{2}) + (iA + \tfrac{1}{2})/2 - (iA + \tfrac{1}{2})^{1/2}\, xe^{-\pi i/4}] \times [1 + O\,|iA|^{-1/2}]. \tag{3.15}$$

If $A = a - iN$, then for $N \gg |a|$, $U(iA, xe^{-\pi i/4})$ becomes an oscillating function whose modulus decreases exponentially like $2^{-1/2}N^{-1/4}\exp[-(N/2)(\ln N - 1) - \sqrt{N/2}\,x]$. If $A = a + iN$ the modulus increases exponentially like $2^{-1/2}N^{-1/4}\exp[(N/2)(\ln N - 1) + \sqrt{N/2}\,x]$. Therefore, to use the recurrence relation (3.12) directly, the starting values should be evaluated at $A = a - iN$, where N is a positive kinteger which depends on a and x. Recurring in the forward direction, the index is raised N times to determine $U(ia, xe^{-\pi i/4})[D_{-ia-1/2}(xe^{-\pi i/4})]$.

In addition to $D_\nu(z)$, other solutions to the recurrence relations (3.1)–(3.3) are $e^{+\nu\pi i}D_\nu(-z)$, $\Gamma(\nu+1)\,e^{\nu\pi i}D_{-\nu-1}(+iz)$. If $A = a - iN$ then $D_{-iA-1/2}(xe^{-\pi i/4})$ decreases exponentially faster than the other solutions to zero as $N \to \infty$ for fixed $x > 0$.

4. Evaluation of $U(a, x)$ and $V(a, x)$

Use of Olver's asymptotic formulas together with the recurrence relations constitutes a convenient and accurate algorithm for the evaluation of the generalized harmonic oscillator functions $U(a, x)$, $V(a, x)$ and their derivatives for wide ranges of both variables. By performing the calculations in double precision arithmetic on a Univac 1182, correct values of the functions and their derivatives are obtained to 14 significant digits. When x is in the neighborhood of the transition point $2\sqrt{-a}$ and a is large and negative, there is a decrease in precision that we will discuss at the end of this section. The choice of the method depends solely on the value of a, which we have divided into two complementary domains:

$a > 40$ or $a < -41$	Asymptotic Region,
$-41 \leqslant a \leqslant 40$	Complementary Region.

When a falls within the asymptotic region, Olver's formulas are employed directly When the functions are needed for non-asymptotic values of a, the asymptotic formulas provide the starting values for the recurrence relations at the large initial indices $a_\pm$. These have been experimentally determined:

$$a_+ = a + N \geqslant 40, \qquad U(a, x),$$
$$a_- = a - M \leqslant -41, \qquad V(a, x).$$

In the case of $U(a, x)$, the function and its derivative, both evaluated at a_+, are first used to obtain $U(a_+ - 1, x)$ from Eq. (3.7). The index is then lowered $N - 1$ times to a employing recurrence relation (3.5) directly backwards. The symmetry of the parabolic cylinder functions with respect to x (see Fig. 1) makes it necessary to develop an algorithm for positive x only. The computational algorithm is summarized in Fig. 4.

For completeness we will now specify which of Olver's asymptotic series are employed in the algorithm and comment on any difficulties that arose in their evaluation. Since we used more terms than Olver originally presented, we have

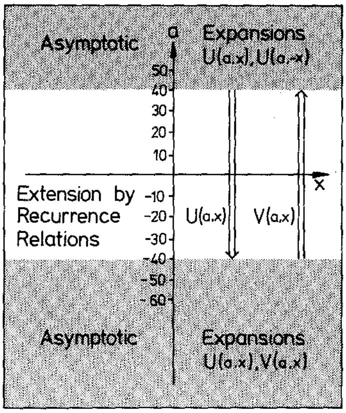

FIG. 4. Computational methods to evaluate $U(a, x)$ and $V(a, x)$ and their derivatives.

recorded the necessary expansion coefficients in Table I (see also the Appendix). The asymptotic representations are derived from an analysis of the normal equation,

$$\frac{d^2}{dt^2} w(\mu, t) = \mu^4(t^2 - 1)\, w(\mu, t), \tag{4.1}$$

where μ and t are complex, and $|\mu| \gg 0$.

For a positive, (4.1) is brought into the form of the real standard differential equation for $U(a, x)$ by the following transformations of the dependent and independent variables: set $t = -iz$, $\mu = i\eta$ and $y(\eta, z) = w(i\eta, -iz)$ to obtain

$$\frac{d^2}{dz^2} y(\eta, z) - \eta^4(z^2 + 1)\, y(\eta, z) = 0, \tag{4.2}$$

and $x = z\eta\sqrt{2}$, $a = \frac{1}{2}\eta^2$, $y(a, x) = y(\sqrt{2a}, x/2\sqrt{a})$ to obtain

$$\frac{d^2}{dx^2} y(a, x) - (\tfrac{1}{4}x^2 + a)\, y(a, x) = 0. \tag{4.3}$$

A satisfactory pair of solutions for (4.3) when a is positive is $U(a, x)$ and $U(a, -x)$. To preserve Olver's notation, the asymptotic formulas are more conveniently written as functions of η and z, and in the following section, we will denote $U(a, x)$ equivalently by $U(\frac{1}{2}\eta^2, z\eta\sqrt{2})$.

Equation (4.3) exhibits no transition point characteristics for real, positive a, and the functions can be expressed in terms of elementary functions [21]:

$$U(a, x) = U\left(\frac{1}{2}\eta^2, \eta z\sqrt{2}\right) \sim \frac{\bar{g}(\eta)\, e^{-\eta^2\bar{\xi}(z)}}{(z^2+1)^{1/4}} \sum_{s=0}^{\infty} \frac{\bar{u}_s(z)}{(z^2+1)^{(3/2)s}} \cdot \frac{1}{\eta^{2s}}, \qquad a > 0, \tag{4.4}$$

TABLE I

Coefficients for the Polynomial Functions $u_s(z)$ and $v_s(z)$ in Common Denominator Form[a]

s	k	D	$u_s ; z^k$	$v_s : z^k$
1	1	24	−6	6
	3		1	1
2	0	1152	145	−143
	2		249	−327
	4		−9	15
3	1	414720	−259290	259290
	3		−151995	238425
	5		−28287	−36387
	7		18189	18189
	9		−4042	−4042
4	0	39813120	12773113	−12118727
	2		122602962	−132752238
	4		50938215	−57484425
	6		−154982	−151958
	8		−321339	551733
	10		72756	−121260
5	1	6688604160	−34009066266	34009066266
	3		−119582875013	130919230435
	5		−37370295816	35213253348
	7		4433574213	3832454253
	9		−3630137104	−3750839308
	11		1994971575	2025529095
	13		−617950920	−617950920
	15		82393456	82393456
6	0	4815794995200	12434112343271	−12052415368249
	2		301898378571021	−311455283274099
	4		586168675568136	−624610264486464
	6		124486509070161	−135687713265279
	8		−1534634176464	2075551573176
	10		414229331745	−774637440975
	12		−244475667255	435211624545
	14		82496447820	−139965883380
	16		−11123116560	18538527600
7	1	115579079884800	−10005934025910666	10005934025910666
	3		−86244319713347575	89579631055317797
	5		−108168741079020387	113744015324794125
	7		−16971937888903074	20079365070264138
	9		−1244028561323341	−1531341334173469
	11		1500261393316578	1514355184823118
	13		−1153987181404935	−1164406579029195
	15		615745509685937	620383849291457
	17		−217738570740306	−218405957733906
	19		45901168957896	45901168957896
	21		−4371539900752	−4371539900752

[a] Ref. [3].

$$U'(a,x) = U'\left(\frac{1}{2}\eta^2, \eta z\sqrt{2}\right)$$
$$\sim \frac{-\eta\bar{g}(\eta)}{\sqrt{2}}(z^2+1)^{1/4}e^{-\eta^2\bar{\xi}(z)}\sum_{s=0}^{\infty}\frac{\bar{v}_s(z)}{(z^2+1)^{(3/2)s}}\cdot\frac{1}{\eta^{2s}}. \tag{4.5}$$

The auxiliary function $\bar{g}(\eta)$ is calculated from the asymptotic expansion

$$\frac{1}{g(\eta)} \sim 2^{(1/4)\eta^2+1/4}e^{+(1/4)\eta^2}\eta^{-(1/2)\eta^2+1/2}\left(1+\sum_{j=0}^{\infty}\frac{g_{2j+1}}{\eta^{4j+2}}\right), \tag{4.6}$$

where $\bar{g}(\eta) = e^{\pi i(1/4+(1/4)\eta^2)}g(i\eta)$, and $\bar{\xi}(z)$ is given by

$$\bar{\xi}(z) = \tfrac{1}{2}z(z^2+1)^{1/2} + \tfrac{1}{2}\ln[z+(z^2+1)^{1/2}]. \tag{4.7}$$

The functions $\bar{u}_s(z)$ and $\bar{v}_s(z)$ are defined in terms of the polynomial functions $u_s(z)$ and $v_s(z)$

$$\begin{aligned}\bar{u}_s(z) &\equiv i^s u_s(-iz),\\ \bar{v}_s(z) &\equiv i^s v_s(-iz).\end{aligned} \tag{4.8}$$

It is a tedious but straightforward exercise to determine the coefficients $u_s(z)$ and $v_s(z)$ from a set of recurrence relations given in the Appendix. We record the coefficients for the first seven functions in Table I [3]. The constants g_s can be obtained from Table I as explained in the Appendix. The branches of the multi-valued functions are well defined upon specifying $\arg\mu = \pi/2$ ($\arg\eta = 0$) and $z\varepsilon e^{\pi i/2}S(\pi/2)$, the domain shown in Fig. 5a. When $x > 0$, Eq. (4.4) is a valid asymptotic representation for the linearly independent solution $U(a, -x)$. The corresponding asymptotic

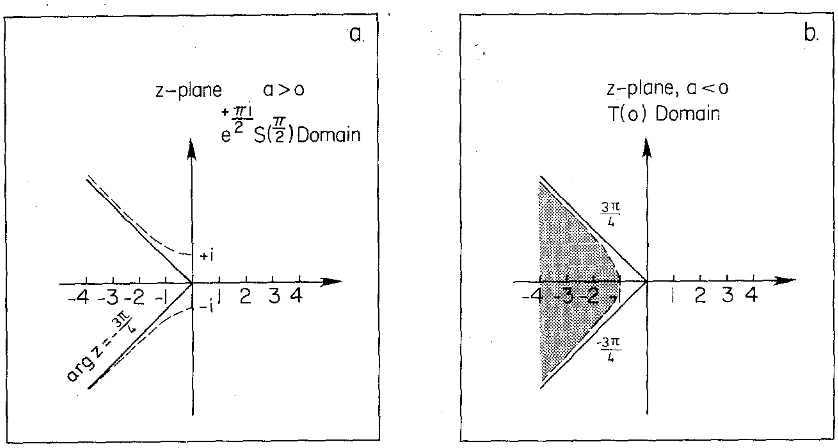

FIG. 5. Domain of asymptotic expansions for (a) $U(\frac{1}{2}\eta^2, \eta z\sqrt{2})$, where $\frac{1}{2}\eta^2 = a$, and (b) $U(-\frac{1}{2}\eta^2, \eta z\sqrt{2})$ and $V(-\frac{1}{2}\eta^2, \eta z\sqrt{2})$, where $\frac{1}{2}\eta^2 = -a$.

formula for $V(a,x)$ can be straightforwardly derived by substitution of the expressions for $U(a,x)$ and $U(a,-x)$ into (2.3).

When a is negative, the change of variables $t=z$, and $\mu=\eta$, followed by $\eta^2=-2a$ and $x=\eta z\sqrt{2}$, again transforms (4.1) into (4.3). However, Eq. (4.3) now possesses two real transition points at $x_{TP}=\pm 2\sqrt{|a|}$. Olver's asymptotic expansions for $U(a,x)$ and $U'(a,x)$, which are uniform for all x to the right of the left hand transition point, are in terms of Airy functions, $Ai(\eta^{4/3}\zeta)$ and $Bi(\eta^{4/3}\zeta)$ [21]:

$$U(a,x)=U\left(\frac{-1}{2}\eta^2,\eta z\sqrt{2}\right)\sim 2\pi^{1/2}\eta^{1/3}g(\eta)\,\Phi(\zeta)$$

$$\times\left\{Ai(\eta^{4/3}\zeta)\sum_{s=0}^{\infty}\frac{A_s(\zeta)}{\eta^{4s}}+\frac{Ai'(\eta^{4/3}\zeta)}{\eta^{8/3}}\sum_{s=0}^{\infty}\frac{B_s(\zeta)}{\eta^{4s}}\right\},\qquad a<0, \qquad (4.9)$$

$$U'(a,x)=U'\left(\frac{-1}{2}\eta^2,\eta z\sqrt{2}\right)\sim\frac{(2\pi)^{1/2}\eta^{2/3}g(\eta)}{\Phi(\zeta)}$$

$$\times\left\{\frac{Ai(\eta^{4/3}\zeta)}{\eta^{4/3}}\sum_{s=0}^{\infty}\frac{C_s(\zeta)}{\eta^{4s}}+Ai'(\eta^{4/3}\zeta)\sum_{s=0}^{\infty}\frac{D_s(\zeta)}{\eta^{4s}}\right\}, \qquad (4.10)$$

where $\Phi(\zeta)=(\zeta/(z^2-1))^{1/4}$. The variable ζ is given by

$$\tfrac{2}{3}\zeta^{3/2}=\tfrac{1}{2}z(z^2-1)^{1/2}-\tfrac{1}{2}\ln(z+(z^2-1)^{1/2})\qquad\text{for}\quad z>1$$

and (4.11)

$$\tfrac{2}{3}(-\zeta)^{3/2}=\tfrac{1}{2}\arccos(z)-\tfrac{1}{2}z(z^2-1)^{1/2}\qquad\text{for}\quad 0\leqslant z<1$$

with $\zeta=0$ at the turning point $z=1$. The coefficient functions [redacted]

$$A_s(\zeta)=\sum_{m=0}b_m\zeta^{-3m/2}\mathscr{A}_{2s-m}(z),\qquad \zeta^{1/2}B_s(\zeta)=-\sum_{m=0}a_m\zeta^{-3m/2}\mathscr{A}_{2s-m+1}(z),$$

(4.12)

$$\zeta^{-1/2}C_s(\zeta)=-\sum_{m=0}^{2s+1}b_m\zeta^{-3m/2}\mathscr{B}_{2s-m+1}(z),\qquad D_s(\zeta)=\sum_{m=0}^{2s}a_m\zeta^{-3m/2}\mathscr{B}_{2s-m}(z),$$

where $\mathscr{A}_0(z)=1$, $\mathscr{A}_s(z)=u_s(z)/(z^2-1)^{3s/2}$, $\mathscr{B}_s(z)=v_s(z)/(z^2-1)^{3s/2}$ and $a_m=(2m+1)(2m+3)\cdots(6m-1)/m!\,(144)^m$, $b_m=-((6m+1)/(6m-1))\,a_m$, with $a_0=1$.

The analogous expansion for $V(a,x)$ follows immediately from Olver's expansion for $\bar{U}(a,x)$ in [21] on dividing by $\Gamma(\frac{1}{2}-a)$.

$$V(a,x)=V\left(\frac{-1}{2}\eta^2,\eta z\sqrt{2}\right)\sim\frac{2\pi^{1/2}\eta^{1/3}g(\eta)}{\Gamma(\frac{1}{2}-a)}\phi(\zeta)$$

$$\times\left\{Bi(\eta^{4/3}\zeta)\sum_{s=0}^{\infty}\frac{A_s(\zeta)}{\eta^{4s}}+\frac{Bi'(\eta^{4/3}\zeta)}{\eta^{8/3}}\sum_{s=0}^{\infty}\frac{B_{s(\zeta)}}{\eta^{4s}}\right\}. \qquad (4.13)$$

$$V'(a,x) = V'\left(\frac{-1}{2}\eta^2, \eta z\sqrt{2}\right) \sim \frac{(2\pi)^{1/2}\eta^{2/3}g(\eta)}{\Gamma(\frac{1}{2}-a)\,\Phi(\zeta)}$$

$$\times\left\{\frac{Bi(\eta^{4/3}\zeta)}{\eta^{4/3}}\sum_{s=0}^{\infty}\frac{C_{s(\zeta)}}{\eta^{4s}} + Bi'(\eta^{4/3}\zeta)\sum_{s=0}^{\infty}\frac{D_s(\zeta)}{\eta^{4s}}\right\}. \qquad (4.14)$$

The multi-valued functions are well defined and the above expressions valid for $z \in T(0)$. $T(0)$ is the unshaded region in Fig. 5b.

As x approaches the right hand transition point $2\sqrt{|a|} = x_{TP}$ or as $z \to 1$ the factor $(\zeta/(z^2-1))^{1/4} \equiv \Phi(\zeta)$ remains well defined and has a finite value at $z=1$. However, evaluation of the series for A_s, B_s, C_s and D_s (Eq. (4.12)) becomes ill-conditioned as x_{TP} is approached. Near $z=1$ the terms in the series, e.g., $b_m\zeta^{-3m/2}\mathscr{B}_{2s-m+1}(z)$ are large with alternating signs, while the series sums are much smaller than the individual terms. The error in the sums becomes worse the larger s is. Since values for the higher derivatives of the Weber functions are easily obtained via the differential equation, the problem is circumvented by applying a Taylor series approximation within the transition region

$$z_1 = 1-\delta_1 < 1 < 1+\delta_2 = z_2.$$

For x within the correponding region, the asymptotic series Eqs. (4.9)–(4.14) are evaluated at z_1, and the numerical integration to the point x is completed using a Taylor series expansion which includes seventh-order derivatives. Use, however, of the Taylor series produces only single precision values of the functions (outside the transition region the algorithm generates double precision values as shown in Table II), and clearly a table of values for $A_s(0)$, $B_2(0)$, $C_s(0)$ and $D_s(0)$ would improve the calculation.

A further problem arises upon evaluating the functions at their zeros using the asymptotic expansions in terms of Airy functions. For large negative a, the functions $U(a,x)$ and $\bar{U}(a,x)$ $[V(a,x)]$ are rapidly oscillating increasing functions when x is between the transition points $\pm 2\sqrt{-a}$, i.e., the classical region. Their magnitude is roughly determined by the factor $2\pi^{1/2}g(\eta)$ in Eqs. (4.9) and (4.13), and asymptotically it behaves like $2^{-1/4-a/2}\Gamma(1/4-a/2)$. Zeros of the functions are obtained when the sums appearing in the brackets are zero. If this sum is not exactly zero a large absolute error will result because of the factor $g(\eta)$. The relative error, e.g., the calculated value of $U(a,x)/U'(a,x)$ at the zeros of $U(a,x)$, does, however, remain small ($<10^{-14}$). This difficulty is most easily remedied by scaling the functions to order unity or by placing a tolerance on the sums for x within the classical region. Since we required only relative values of $U(a,x)$ and $\bar{U}(a,x)$ at different values of x for fixed a, we omitted the factor $g(\eta)$ thereby altering the normalization.

The accuracy of the calculated functions was determined by a variety of methods. To obtain double precision accuracy for small x, it is necessary to include eight terms ($s=7$) in the elementary function expansions (4.4) and (4.5) and four terms ($s=3$) in the Airy function expansions (4.9), (4.10), (4.13), and (4.14). For large x, the

TABLE II

Comparison of Computed to Exact[a] Values at $U(-n-1/2, x)$

x	$U(-2.5, x)$	$U(-5.5, x)$	$U(-10.5, x)$
0	−1.00000000000003 −1.00000000000000	0.0000000000000 0.0000000000000	(+2) −9.45000000000023 (+2) −9.45000000000000
1	0.0000000000000 0.0000000000000	4.67280469842844 4.67280469842843	(+2) 9.47021752214830 (+2) 9.47021752214828
5	(−2) 4.63308992694651 (−2) 4.63308992694650	3.76438556564404 3.76438556564403	(+2) 3.46863999197395 (+2) 3.46863999197395
10	(−9) 1.37490644263144 (−9) 1.37490644263144	(−6) 1.25199813942651 (−6) 1.25199813942651	(−2) 8.47021745898525 (−2) 8.47021745898523
20	(−41) 1.48431031443232 (−41) 1.48431031443231	(−37) 1.16077530679778 (−37) 1.16077530679778	(−31) 3.39561760425668 (−31) 3.39561760425668

[a] The exact values, obtained from Tables 22.12 and 22.13 in [1], are written below the computed values.

same precision is possible using fewer terms. For fixed a, evaluation of the Wronskian

$$W\{U(a,x), V(a,x)\} = (2/\pi)^{1/2}$$

or

$$W\{U(a,x), \bar{U}(a,x)\} = (2/\pi)^{1/2}\,\Gamma(\tfrac{1}{2}-a) \qquad \text{for} \quad a \leqslant 0$$

$$W\{U(a,x), U(a,-x)\} = (2\pi)^{1/2}/\Gamma(a+\tfrac{1}{2}) \qquad \text{for} \quad a \geqslant 0$$

as a function of x shows the double asymptotic nature of Olver's expansions, i.e., the accuracy increases with increasing x and a. For $x=0$, the calculated values of $U(a,0)$ and $V(a,0)$ were compared to the analytic expressions in [1]:

$$U(a,0) = \frac{\sqrt{\pi}}{2^{a/2+1/4}\,\Gamma(3/4+a/2)},$$

$$V(a,0) = \frac{2^{a/2+1/4}\sin\pi(3/4-a/2)}{\Gamma(3/4-a/2)}.$$

The zeros of the functions $U(a,0)$ and $V(a,0)$ can easily be obtained from these expressions and serve as an additional check. For small x and a, the computed values were in agreement to all places with the values given in the 5-figure tables for $U(a,x)$ and $V(a,x)$ in [1] and the 8-figure tables for $U(a,x)$ in [13]. When a is a negative half-integer, $U(-n-\frac{1}{2}, x)$ can be expressed in terms of the Hermite polynomials

$H_n(x/\sqrt{2})$ (see Eq. (2.4)). Table II shows a comparison of the computed to the exact values. The range of x over which the algorithm can be applied is determined by the argument of the Airy functions in the asymptotic expansions, e.g., $Ai(\eta^{4/3}\zeta)$. For large positive x, $\eta^{4/3}\zeta$ is essentially independent of a, and $Ai(\eta^{4/3}\zeta)$ behaves approximately like $e^{-x^2/4}$. To implement the algorithm on a Univac 1182, one must limit x to the region $0 \leqslant x \leqslant 45$.

5. Evaluation of $W(a, x)$ and $E(a, x)$

As with the functions $U(a, x)$ and $V(a, x)$, one would like to use Olver's uniform asymptotic series to evaluate $k^{\mp 1/2}W(a, \pm x)$ or $E(a, x)$ for large magnitudes of a and devise a recursion scheme, which is dependent on a only, x being treated as a parameter, to cover the complementary region of non-asymptotic values of a:

$$\begin{array}{ll} a < -40 \text{ or } a > 20 & \text{Asymptotic Region,} \\ -40 \leqslant a \leqslant 20 & \text{Complementary Region.} \end{array} \tag{5.1}$$

We have already outlined such a scheme in Section 3 involving the complex recurrence relations for $U(iA, xe^{-\pi i/4})$, where $A = a - iN$. For large values of the complex parameter A, Olver has developed asymptotic series for $U(iA, z)$ and its derivative which are uniformly valid with respect to the z variable. For a in the complementary region and $z = xe^{-\pi i/4}$, these complex asymptotic series are used to generate values of $U(iA, z)$ and $U'(iA, z)$ at $A = a - iN$ which are subsequently employed in the recurrence relation (3.14) to obtain $U(i(A + i), z)$. The direct forward recurrence of Eq. (3.12) $N - 1$ times produces $U(ia, z)$, and $U'(ia, z)$ is determined at the end from Eq. (3.13). Substitution of $U(ia, xe^{-\pi i/4})$ into Eq. (2.8) gives the desired function $E(a, x)$.

Olver's expansions for $U(iA, xe^{-\pi i/4})$ and $W(a, \pm x)$ are derived from the normal equation

$$\frac{d^2}{dt^2} w(\mu, t) = \mu^4(t^2 - 1)\, w(\mu, t) \tag{5.2}$$

in which μ and t are complex variables. The following change of variables transforms (5.2) into the desired form: set $t = -iz$, $\eta = e^{-i\pi/4}\mu$, and $y(\eta, z) = w(\eta e^{+\pi i/4}, -iz)$ to obtain

$$\frac{d^2}{dz^2} y(\eta, z) = -\eta^4(z^2 + 1)\, y(\eta, z) \tag{5.3}$$

and $x = \eta z\sqrt{2}$, $A = -\frac{1}{2}\eta^2$, $y(A, x) = y(\sqrt{-2A}, x/2\sqrt{-A})$ to obtain

$$\frac{d^2}{dz^2} y(A, x) = -(\tfrac{1}{4}x^2 - A)\, y(A, x). \tag{5.4}$$

As stated in Section 2, the principal solution of Eq. (5.4) is $U(iA, xe^{-\pi i/4})$ where we have made use of Miller's notation

$$U(iA, z) = D_{-iA-1/2}(z). \tag{5.5}$$

When A takes on complex values, $A = a - iN$, (5.4) exhibits no real transition point characteristics, and the asymptotic series for $U(iA, xe^{-\pi i/4})$ can be expressed in terms of elementary functions. The expansions when Re(A) is negative are [21]

$$U(iA, xe^{-\pi i/4}) = U\left(\frac{-i\eta^2}{2}, e^{-\pi i/4} z\eta\sqrt{2}\right) \sim \frac{g(\eta e^{\pi i/4})\, e^{\eta^2(i\xi(z)+\pi/4}}{(z^2+1)^{1/4}\, e^{-\pi i/4}} \cdot \sum_{s=0}^{\infty} (-1)^s \frac{u_s(-iz)}{(z^2+1)^{(3/2)s}} \cdot \frac{1}{\eta^{2s}} \tag{5.6}$$

and

$$U'\left(\frac{-i\eta^2}{2}, e^{-\pi i/4}\eta z\sqrt{2}\right) \sim \frac{-\eta}{2}\, g(\eta e^{\pi i/4})(z^2+1)^{1/4}\, e^{\eta^2(i\xi(z)+\pi/4)}\, e^{-\pi i/4} \cdot \sum_{s=0}^{\infty} \frac{(-1)^s v_s(-iz)}{(z^2+1)^{(3/2)s}} \cdot \frac{1}{\eta^{2s}}. \tag{5.7}$$

The functions $g(\eta)$, $\xi(z)$ are as defined in the previous section. The polynomial functions $u_s(z)$ and $v_s(z)$ are given in the Appendix and their expansion coefficients for $s \leqslant 7$ are recorded in Table I [3]. The region of validity of the above expression is $z \in e^{\pi i/2} S(\arg\mu)$, where $\arg\mu$ varies with N as follows:

$$0 \leqslant N < \infty,$$

$$0 \leqslant \arg\eta < \frac{\pi}{4}, \qquad \text{where} \qquad -\frac{1}{2}\eta^2 = a - iN,\ a < 0, \tag{5.8}$$

$$\frac{\pi}{4} \leqslant \arg\mu < \frac{\pi}{2}.$$

[illegible]

which lead to asymptotic series for $U(iA, e \ldots x)$ is

$$\eta = e^{\pi i/4}\mu, \qquad z = t,$$
$$x = \eta z\sqrt{2}, \qquad A = \tfrac{1}{2}\eta^2. \tag{5.9}$$

The series expansions in terms of these redefined variables are [21]

$$U\left(\frac{i\eta^2}{2}, e^{-\pi i/4}\eta z\sqrt{2}\right) \sim \frac{g(\eta e^{-\pi i/4})\, e^{i\eta^2\xi}}{(z^2-1)^{1/4}} \sum_{s=0}^{\infty} i^s \frac{u_s(t)}{(z^2-1)^{(3/2)s}} \cdot \frac{1}{\eta^{2s}}, \tag{5.10}$$

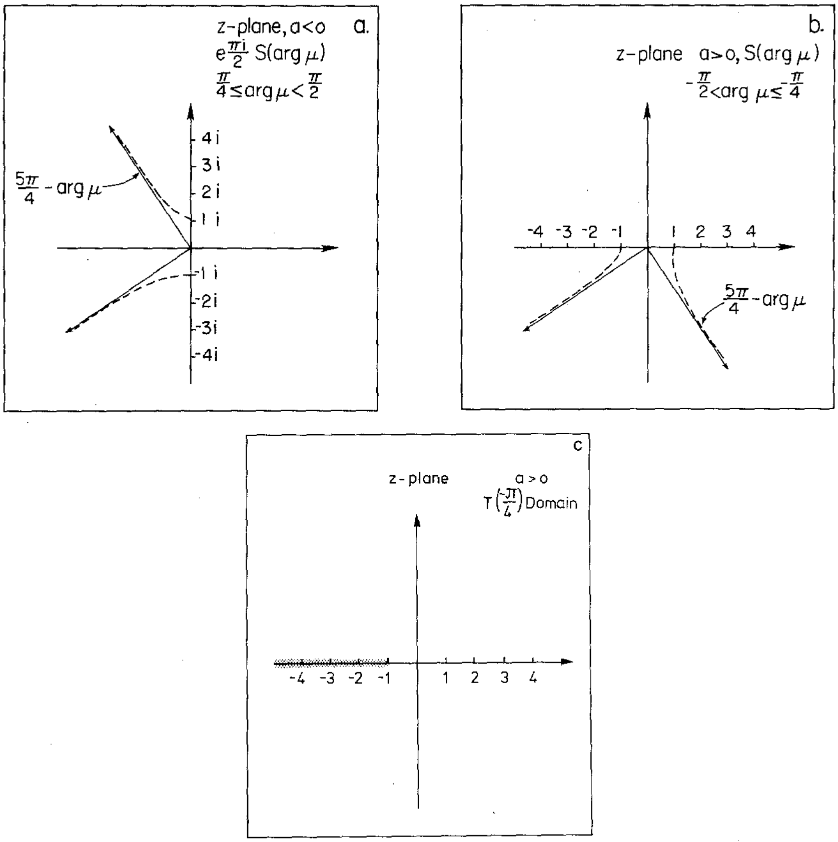

FIG. 6. Domain of asymptotic expansions for (a) $U(-i\eta^2/2, \exp(-i\pi/4)\, z\eta\sqrt{2})$ and (b) $U(i\eta^2/2, \exp(-i\pi/4)\, z\eta\sqrt{2})$. (c) Domain of asymptotic expansions for $W(\frac{1}{2}\eta^2, \pm\eta z\sqrt{2})$.

$$U'\left(\frac{i\eta^2}{2}, e^{-\pi i/4}\eta z\sqrt{2}\right) \sim \frac{-\eta}{\sqrt{2}}\, g(\eta e^{-\pi i/4})(z^2-1)^{1/4}\, e^{i\eta^2\xi} \sum_{s=0}^{\infty} \frac{i^s v_s(t)}{(z^2-1)^{(3/2)s}} \cdot \frac{1}{\eta^{2s}}, \quad (5.11)$$

where $\xi(z) = \frac{1}{2}z(z^2-1)^{1/2} - \frac{1}{2}\ln[z + (z^2-1)^{1/2}]$.

The range of the arguments of η and μ as a function of N are

$$0 \leqslant N < \infty,$$

$$0 \geqslant \arg\eta > \frac{-\pi}{4}, \qquad \text{where} \qquad \frac{1}{2}\eta^2 = a - iN,\ a \geqslant 0, \quad (5.12)$$

$$\frac{-\pi}{4} \geqslant \arg\mu > \frac{-\pi}{2}.$$

The branch cuts that define the multi-valued function $\xi(z)$ and form the boundaries of the domain $S(\arg\mu)$ are labeled in Fig. 6b.

Evaluation of the complex function $U(iA, xe^{-\pi i/4})$ for subsequent use in the recurrence relations with a complex index is only necessary when the energy parameter a lies within the complementary region defined in (5.1). When $a < -40$, the functions $k^{\mp 1/2}W(a, \pm x)$ can be evaluated directly from the components of $E(a, x)$ (A real) using (2.7), (2.8) and (5.6). When a lies in the positive asymptotic range, $a \geqslant 40$, $k^{\mp 1/2}W(a, \pm x)$ and their derivatives are computed by Olver's real uniform asymptotic series in terms of Airy functions:

$$W(a, x) = W\left(\frac{1}{2}\eta^2, \eta z\sqrt{2}\right) \sim \frac{\pi^{1/2}\eta^{1/3}l(\eta)}{2^{1/2}e^{\pi\eta^2/4}}\left(\frac{\zeta}{z^2-1}\right)^{1/4}$$
$$\times \left\{Bi(-\eta^{4/3}\zeta)\sum_{s=0}^{\infty}(-)^s\frac{A_s(\zeta)}{\eta^{4s}} + \frac{Bi'(-\eta^{4/3}\zeta)}{\eta^{8/3}}\sum_{s=0}^{\infty}(-)^s\frac{B_s(\zeta)}{\eta^{4s}}\right\}, \tag{5.13}$$

$$W'(a, x) = W'\left(\frac{\eta^2}{2}, \eta z\sqrt{2}\right) \sim \frac{\pi^{1/2}\eta^{2/3}l(\eta)}{2e^{\pi\eta^2/4}}\left(\frac{z^2-1}{\zeta}\right)^{1/4}$$
$$\times \left\{\frac{Bi(-\eta^{4/3}\zeta)}{\eta^{4/3}}\sum_{s=0}^{\infty}(-)^s\frac{C_s(\zeta)}{\eta^{4s}} - Bi'(-\eta^{4/3}\zeta)\sum_{s=0}^{\infty}(-)^s\frac{D_s(\zeta)}{\eta^{4s}}\right\}, \tag{5.14}$$

$$W(a, -x) = W\left(\frac{\eta^2}{2}, -\eta z\sqrt{2}\right) \sim \frac{\pi^{1/2}\eta^{1/3}l(\eta)}{2^{-1/2}e^{-\pi\eta^2/4}}\left(\frac{\zeta}{z^2-1}\right)^{1/4}$$
$$\times \left\{Ai(-\eta^{4/3}\zeta)\sum_{s=0}^{\infty}(-)^s\frac{A_s(\zeta)}{\eta^{4s}} + \frac{Ai'(-\eta^{4/3}\zeta)}{\eta^{8/3}}\sum_{s=0}^{\infty}(-)^s\frac{B_s(\zeta)}{\eta^{4s}}\right\}, \tag{5.15}$$

$$W'(a, -x) = W'\left(\frac{\eta^2}{2}, -\eta z\sqrt{2}\right) \sim \frac{\pi^{1/2}\eta^{2/3}l(\eta)}{e^{-\pi\eta^2/4}}\left(\frac{z^2-1}{\zeta}\right)^{1/4}$$
$$\times \left\{\frac{Ai(-\eta^{4/3}\zeta)}{\eta^{4/3}}\sum_{s=0}^{\infty}(-)^s\frac{C_s(\zeta)}{\eta^{4s}} - Ai'(-\eta^{4/3}\zeta)\sum_{s=0}^{\infty}(-)^s\frac{D_s(\zeta)}{\eta^{4s}}\right\}, \tag{5.16}$$

where $W'(a, -x) = dW(a, -x)/dx$ and $l(\eta) \equiv 2^{1/2}e^{\pi\eta^2/8}e^{i(\phi(a)/2-\pi/8)}g(\eta e^{-\pi i/4})$ with the $\phi(a) = \arg\Gamma(\frac{1}{2}+ia)$ (see Section 2).

The expansions are valid for z in the region $T(-\pi/4)$, where $\arg\mu = -\pi/4$ and $\arg\eta = 0$ (Fig. 6c).

The expansions coefficients $A_s(\zeta)$, $B_s(\zeta)$, $C_s(\zeta)$ and $D_s(\zeta)$ are evaluated by the series given in Eq. (4.12). As explained in Section 4, these series become ill-conditioned as the transition point (here $x_{TP} = 2\sqrt{a}$) is approached. Near $z = 1$, there are heavy cancellations in the sums which become worse the larger s is. Again the difficulty is circumvented by employing a Taylor series approximation to the Weber functions when x is in the neighborhood of a transition point. Use, however, of the Taylor series produces function values at x_{TP} which are the least accurate in the entire algorithm (8 vs 11 significant digits), and clearly a table of values for $A_s(0)$, $B_s(0)$, $C_s(0)$, and $D_s(0)$ would improve the evaluation.

The asymptotic series for $W(a, \pm x)$ and $W'(a, \pm x)$ [Eqs. (5.13)–(5.16)] have variable accuracy over the asymptotic region, as was determined from evaluating the Wronskian and spot-checking against expansions for large and small x found in the NBS handbook [1]. The accuracy of calculations performed with double precision arithmetic on a Univac 1182, expressed as significant digits, is indicated in Fig. 7 for the three term ($s \leqslant 2$) and four term ($s \leqslant 3$) series. The accuracy increases with increasing x since $\lim_{x\to\infty} A_s \to 0$ for $s > 1$ and $\lim_{x\to\infty} B_s \to 0$. At the origin, the coefficients A_s, B_s, C_s, D_s are of order 1, e.g., $A_s(t=0) = \sum_{m=0}^{s} b_{2m} \zeta_{(0)}^{-3m} \mathscr{A}(0)_{2s-2m}$, and the asymptotic series, truncated at the jth term, are correct to $O[1/(2a)^{2j+2}]$.

When a is in the negative portion of the complementary region (5.1), the above algorithm with $s=6$ in Eqs. (5.6) and (5.7) [e.g., the series includes terms up to U_6 and V_6, and $j=2$ in the series for $g(\eta)^{-1}$ Eq. (4.6)] generates better than single precision values of $E(a,x)$ or equivalently $k^{\pm 1/2} W(a, \pm x)$. The number of steps needed for the recurrence process as a function of a and x is given in Table III. For a in the positive portion of the complementary region, similar accuracy is obtained except when x is in the limited range $0 \leqslant x \leqslant x_{TP} = 2\sqrt{a}$ (e.g., x in the so-called non-classical or exponential region). For $x < x_{TP}$ numerical difficulties exist in determining the imaginary part of $E(a,x)$ from $U(ia, xe^{-\pi i/4})$ which is obtained from the recurrence relations. The problem arises from the disparity in size between the real and imaginary components of $E(a,x)$ (see Fig. 1e),

$$\frac{\operatorname{Re} E(a,x)}{\operatorname{Im} E(a,x)} = \frac{k^{-1/2} W(a,x)}{k^{1/2} W(a,-x)} \sim 2e^{\pi a}, \qquad a > 0,\ 0 \leqslant x \ll x_{TP}.$$

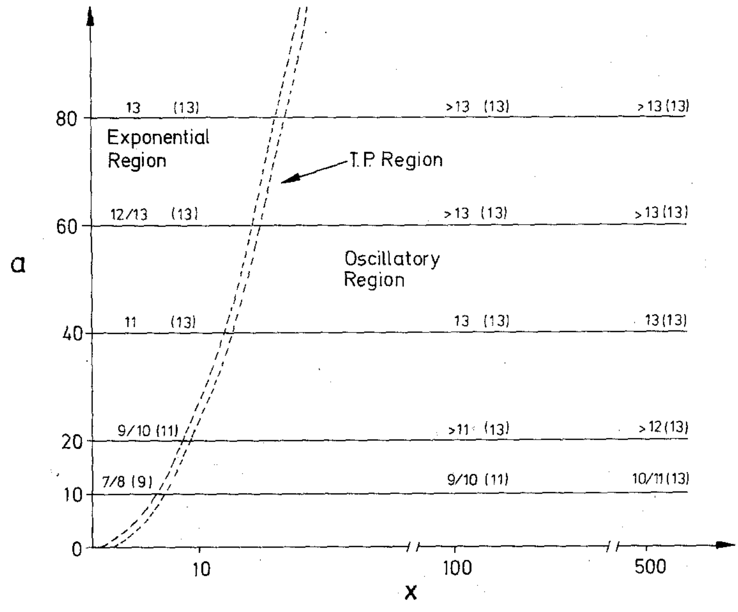

FIG. 7. Accuracy (number of significant digits) of 3 (4) term asymptotic series for $W(a, \pm x)$, $a > 0$, Eqs. (5.13) and (5.15).

TABLE III

Recurrence Index N for $U(iA, xe^{-\pi i/4})^a$, $A = a - iN$

a	x	N
$-40 < a < 20$	$0 \leqslant x \leqslant 20$	60
	$20 \leqslant x \leqslant 100$	10
$-40 < a < 4$	$100 < x \leqslant 200$	10
$-2 \leqslant a \leqslant 2$	$200 < x \leqslant 500$	4

[a] $U(iA, xe^{-\pi i/4})$ is evaluated from Eq. (5.6) for $a < 0$ and Eq. (5.10) for $a > 0$, using $s = 6$. $g(\eta)$ is determined from Eq. (4.6) with $j = 2$.

Near the origin, the phase of $E(a, x)$ is extremely small while the phase of $U(ia, xe^{-\pi i/4})$ is approximately $-\pi/8 - \phi/2$ (see (2.7) and (2.8)). Round-off error due to the almost complete cancellations of the phases between $U(ia, xe^{-\pi i/4})$ and the pre-factors, leads to loss of accuracy in evaluation of Im $E(a, x)$.

There are a number of ways to circumvent this problem. Our solution is to employ the complex recurrence relations in the exponential region, $0 \leqslant x \leqslant 2\sqrt{a}$, to obtain just the dominant real component $k^{-1/2}W(a, x)$ and $k^{-1/2}W'(a, x)$. The ratio $W'(a, -x)/W(a, -x) = y$ can be evaluated from Miller's [18] non-linear differential equation for the derivative-log function,

$$\frac{dy}{dx} + y^2 + 1/x^2 - a = 0,$$

where

$$y_0 = \frac{W'(a, 0)}{W(a, 0)} = -2^{1/2} \frac{|\Gamma(\frac{3}{4} + \frac{1}{2}ia)|}{|\Gamma(\frac{1}{4} + \frac{1}{2}ia)|},$$

using fourth-order Runge–Kutta integration with stepsizes $\leqslant 0.005$. From the Wronskian relation

$$W(a, x)\frac{W'(a, -x)}{W(a, -x)} - W'(a, x) = \frac{1}{W(a, -x)}$$

one can solve for $W(a, -x)$ and subsequently $W'(a, -x)$ in a numerically stable fashion.

The computational methods to evaluate at least single precision values [values correct to at least eight significant digits] of the parabolic cylinder functions $k^{\mp 1/2}W(a, \pm x)$ and their derivatives are summarized in Fig. 8. The calculations were performed using double precision arithmetic on a Univac 1182. Within the exponential region $0 \leqslant x \leqslant 2\sqrt{a}$, for $1 < a < 20$ only the functions $k^{-1/2}W(a, x)$ and $k^{-1/2}W'(a, x)$ are obtained from the complex recurrence relations for $E(A, x)$. The

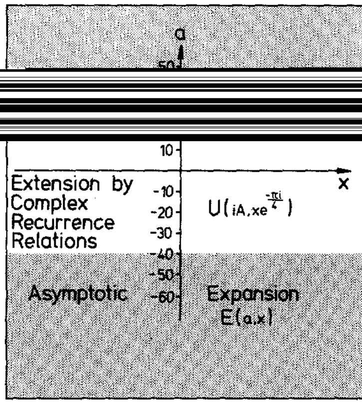

FIG. 8. Computational methods to evaluate $k^{\mp 1/2}W(a, \pm x)$ and their derivatives.

imaginary components $k^{1/2}W(a, -x)$ and $k^{+1/2}W'(a, -x)$ are discarded and determined instead from Miller's derivative-log method discussed above.

The accuracy of the algorithm when a is in the complementary region was determined by monitoring the Wronskian $W\{W(a, x), W(a, -x)\}$ and by comparing the function values to existing tables and expansions. For small x, the computed values agree to all places given in Miller's 9-figure tables of $W(a, \pm x)$ [18]. For small $|a|$

TABLE IV

Comparison of Computed to Exact[a] Values of $W(a, \pm x)$

a	$W(a, 0)$[b]	$W(a, 250)$[c]	$W(a, -250)$[c]
−2	(−1) 6.0027462289575	(−2) −1.3602243109050	(−2) −8.8480095155775
	(−1) 6.0027462289575	(−2) −1.3602243109048	(−2) −8.8480095155776
−1	(−1) 7.3148109024543	(−2) +6.2184466092715	(−2) −6.4319823309571
	(−1) 7.3148109024543	(−2) +6.2184466092718	(−2) −6.4319823309568
0	1.0227656721132	(−2) +5.0615076282762	(−2) −6.6196245716256
	1.0227656721131	(−2) +5.0615076282764	(−2) −6.6196245716251
1	(−1) 7.3148109024542	(−2) +1.2849662395742	(−1) −1.2820788333744
	(−1) 7.3148109024543	(−2) +1.2894662395742	(−1) −1.2820788333741
2	(−1) 6.0027462289575	(−3) +2.0353322718464	1.9536775486873
	(−1) 6.0027462289575	(−3) +2.0353322718463	1.9636775486873

[a] Exact values are listed below the computed values.
[b] The exact values are from Eq. (19.17.4) in [1].
[c] The exact values are from Miller's asymptotic expansions for modulus and phase, Eqs. (345)–(360) in [18].

and large x, i.e., $x^2 \gg 4a$, a region in which $k^{\mp 1/2} W(a, \pm x)$ are oscillating functions, the values have been checked against the Miller's modulus-phase expressions [1, 18]:

$$k^{-1/2} W(a, x) + ik^{1/2} W(a, -x) = Fe^{i\chi},$$
$$k^{-1/2} W'(a, x) + ik^{1/2} W'(a, -x) = Ge^{i\psi}.$$

A typical comparison is shown in Table IV. For $0 < |a| \leqslant 4$, $x > 200$, Olver's exponential expansions, Eqs. (5.6), (5.7) and Eqs. (5.10), (5.11) with $N \leqslant 4$ agree with Miller's expressions to at least 11 significant digits. Such an agreement is not surprising since Olver has shown in [23] that his expansions for $U(a, x)$ have a double asymptotic property, one for large a and one for large x.

Appendix: Evaluation of Coefficients for Asymptotic Representations of Weber's Parabolic Cylinder Functions

The coefficient functions u_s and v_s in the asymptotic series representation of $U(a, x)$ for $a > 0$ and $E(A, x)$ for complex A are either totally even or odd polynomials of maximum degree $3s$. We shall denote the argument of u_s and v_s generally by z and evaluate them by a set of recurrence formulas [21].

The recurrence formula for $u_s(z)$ given in (4.8) is

$$(z^2 - 1)\, u_s'(z) - 3szu_s(z) = r_{s-1}(z), \tag{A.1}$$

where

$$8r_s(z) = (3z^2 + 2)\, u_s(z) - 12(s+1)\, zr_{s-1}(z) + 4(z^2 - 1)\, r_{s-1}'(z) \tag{A.2}$$

and $u_0(z) = 1$.

The functions $r_s(z)$ are determined first from Eq. (A.2) and then substituted into (A.1). Since the coefficient functions $u_s(z)$ are polynomials of degree $3s$, they can be derived from Eq. (A.1) by matching powers of z. For s even, the coefficients of the leading term z^{3s} in $u_s(z)$ are zero.

Once $u_s(z)$ and $r_s(z)$ are known, the coefficient function $v_s(z)$ is evaluated from the relation

$$v_s(z) = u_s(z) + \tfrac{1}{2} zu_{s-1}(z) - r_{s-2}(z), \tag{A.3}$$

where $v_0(z) = 1$.

Olver provided the functions $u_s(z)$ and $v_s(z)$ for $s = 0, 1, 2, 3$. In order to increase the accuracy of the asymptotic series for moderate values of a, at least two more terms should be included. In Table I we have recorded the coefficients for the polynomials for $s = 1, 2, \ldots, 7$, obtained from solving (A.1)–(A.3).

The constants g_s appearing in (4.6) are defined to be

$$g_s = \lim_{|z|\to\infty} \frac{u_s(z)}{(z^2-1)^{(3/2)s}}.$$

Hence $g_{2s}=0$ and g_{2s+1} is the coefficient of the leading power z^{6s+3} in $u_{2s+1}(z)$ and can be obtained from Table I.

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