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On the Calculation of the Parabolic Cylinder Functions*

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An integral representation for the parabolic cylinder functions is solved by Gaussian quadrature employing an algorithm due to Gordon for solution of the moment equations. This method provides the function $U(a, x)$ for a range of the arguments a and x not previously accessible with the accuracy of the present work.

I. INTRODUCTION

In recent years there has been some interest shown in obtaining solutions to the Schroedinger equation appropriate to various problems by techniques of numerical integration [1, 2, 3]. Of particular interest to us is the problem of solving coupled differential equations [4] for which Gordon [5] has recently developed a method involving a polynomial approximation to the "potential" function rather than to the "wavefunction" as is the case, for example, in the Numerov–Cooley technique [6]. This reference potential is chosen within each interval throughout the region of integration in such a way that the corresponding Schroedinger equation has two linearly independent exact solutions whose form depends on the degree of the approximating polynomial. For example, a constant reference potential corresponds to trigonometric solutions, a linear potential to Airy functions, a quadratic potential to parabolic cylinder functions, etc. The wavefunction associated with the Schroedinger equation containing the true potential over a given interval is an appropriately chosen linear combination of these reference solutions. Prerequisite to obtaining solutions for the problem in question, then, is the accurate calculation of the special functions comprising the reference solutions.

Much of the attention has been focused on the linear reference potential, for which reference solutions are expressed in terms of the Airy functions [5]. A more accurate representation of the true potential would be an quadratic reference potential for which the parabolic cylinder functions serve as reference solutions.

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As Gordon [7] has recently emphasized, while these functions may be calculated for small and large values of the arguments by power series and asymptotic methods [8], respectively, there are regions of the arguments for which no adequate solutions are available. In this paper we report a method for calculating one of the two linearly independent parabolic cylinder functions for a particular range of argument. The general approach is outlined in Section II. Some representative results with a discussion are included in Section III.

II. Theory

The parabolic cylinder functions, or Weber functions, satisfy the differential equation

$$y''(x) = [(1/4)\, x^2 + a]\, y(x). \tag{1}$$

Linearly independent solutions to this equation, labeled $U(a, x)$ and $V(a, x)$, are linear combinations of the even and odd solutions obtained by the usual power series method. An integral representation [9] for $U(a, x)$ may be written in the form

$$U(a, x) = \frac{e^{(-1/4)x^2}}{x^{a-(1/2)}\Gamma[a + (1/2)]} \int_0^\infty \frac{\rho(z)\, dz}{(z^2 + x^2)^{1/2}}, \tag{2}$$

where the weight function $\rho(z)$ is

$$\rho(z) = e^{(-1/4)z^2} z^{a-(1/2)}\, U(-a, z). \tag{3}$$

The moments of the weight functions are given as [10]

$$\mu_k = \int_0^\infty x^k \rho(z)\, dz = \pi^{1/2} 2^{-k/2} \Gamma(k + a + 1/2)/\Gamma[(1/2)k + 1/2]. \tag{4}$$

Equation (2) is restricted to values of $a > (-1/2)$ and Eq. (4) must have $a + k > (-1/2)$. This second restriction allows a value of $k = 0$, since a must always exceed $(-1/2)$, so that all moments μ_k, $k = 0, 1, 2, \ldots$, may be calculated from Eq. (4).

In order that Eq. (2) be valid the denominator in the integral must be analytic and the weight function positive over the range of integration. The former is satisfied for positive z; the latter depends on the sign of $U(-a, z)$ which is positive [11] for allowable values of a less than about 1.8. One can therefore evaluate the integral in Eq. (2) by a method analogous to that described by Gordon [5] for the Airy functions, in which the integral is approximated as a sum

$$U(a, x) = \frac{e^{(-1/4)x^2}}{x^{a-(1/2)}\Gamma[a + (1/2)]} \sum_{i=1}^{n} \frac{w_i^{(b)}}{[(z_i^{(b)})^2 + x^2]^{1/2}}, \qquad b = e, 0, \tag{5}$$

where (b) denotes the even or odd approximant as defined in the algorithm described by Gordon [12] for solving the moment equations. The value of $U(a, x)$ is taken to be the average of the even and odd approximants.

Because the value of a allowed by this procedure has a lower bound at $(-1/2)$, it is useful to obtain the derivative of the parabolic cylinder function so that recurrence relations [13] may be used to evaluate the function for values of a beyond this limit. Algebraic manipulation yields the equations:

$$U(a-1, x) = (1/2)x\, U(a, x) - U'(a, x), \tag{6}$$

$$U(a+1, x) = -[a + (1/2)]^{-1}[U'(a, x) + (1/2)x\, U(a, x)]. \tag{7}$$

These equations may then be substituted into another recurrence relation

$$xU(a, x) - U(a-1, x) + [a + (1/2)]\, U(a+1, x) = 0 \tag{8}$$

to extend the possible values of a for which the function may be calculated.

The method described above may conveniently be used to calculate values of the derivative. Differentiation of Eq. (2) with respect to x gives

$$U'(a, x) = \frac{-e^{(-1/4)x^2}}{x^{a-(1/2)}\Gamma[a + (1/2)]} \times \left\{ \left[\frac{a-(1/2)}{x} + (1/2)x\right] \int_0^\infty \frac{\rho(z)\, dz}{(z^2 + x^2)^{1/2}} + x \int_0^\infty \frac{\rho(z)\, dz}{(z^2 + x^2)^{3/2}} \right\}. \tag{9}$$

Note that the first integral in this expression is identical to that in Eq. (2), while the second integral differs only by the exponent in the denominator. This second integral still satisfies the criteria given earlier, since the weight function is unchanged and the denominator is an analytic function. These integrals can therefore be evaluated according to the method used for Eq. (2), and the calculation of the derivative is accomplished in the same range of a as the function.

III. Results and Discussion

The method described above for calculating the parabolic cylinder function $U(a, x)$ was programmed for the NTSU/IBM 360-50 computer, with all calculations being carried out in double precision. Representative results are displayed in Tables I and II for $a = -0.4$ and $a = +0.6$, respectively, with x ranging from $x = 0.2$ to $x = 16.0$. For comparison we also show the values obtained from the National Bureau of Standards (NBS) tables [11] wherever possible (the NBS tables only go to $x = 5.0$). The underlined values indicate the onset of good agreement with the tabulated values in going from small to large x. Also shown are the derivatives $U'(a, x)$, from which the entries in the columns labeled $U(a - 1, x)$ and $U(a + 1, x)$ were calculated via Eqs. (6) and (7), respectively. The errors listed in column 4 of each table are calculated as one-half the difference between the odd and even approximants to the function in Eq. (5). In accordance with the algorithm of Gordon [12], the integral representation in Eq. (2) is bounded above by the even approximant and below by the odd approximant, so that the error is expressed as one-half the difference between the upper and lower bounds. Note that this difference decreases as x becomes large for fixed a.

As shown in Tables I and II, this method is not accurate for small values of the argument x because of the small x-dependent terms in the denominators of Eq. (5). Near the origin, the moments in the sum do not compensate for the small terms in the denominator, resulting in poor convergence. However, this is not a serious handicap because the power series expansions [8] give extremely accurate values of the function for small x, allowing one to supplement the present method with power-series solutions for these ranges of the argument.

It was mentioned in Section II that the parabolic cylinder function $U(-a, x)$ in the weight function (Eq. (3)) must be positive definite in order that Eq. (2) be valid, implying that a not exceed a value of about 1.8 [11]. However, our experience has shown that for values of a greater than about 0.7 the results for $U(a, x)$ become erratic. Essentially, this is due to the fact that the gamma function in the numerator of Eq. (4) becomes large for larger values of a; the corresponding moments μ_k are used in the form of products in the matrix formalism of Gordon's algorithm and only the lower moments yield accurate results. In practice we were able to use the first five moments for a range of $-0.5 < a < 0.8$, and the results in Tables I and II were calculated in this way.

The range of a for which good solutions are obtainable may be extended by use of the recurrence relations (Eq. (6) and (7)), since the derivative $U'(a, x)$ may be calculated in the same manner as $U(a, x)$. This may be seen from Eq. (9), where the weight function $\rho(z)$ in the two integrals is the same as that in Eq. (2). Thus, a series approximation analogous to Eq. (5) may be employed for $U'(a, x)$, enabling accurate values of $U(a, x)$ to be calculated for $-1.5 < a < 1.8$. The values of the derivatives as well as the recurrence values $U(a + 1, x)$ and $U(a - 1, x)$ are included in the tables.

In principle, one could use the recurrence relations repeatedly to extend the range of a even further. However, one can see from Eq. (8) that the coefficients of $U(a, x)$ and $U(a + 1, x)$ would tend to magnify any erors in these functions, and in practice it is found that accurate solutions via the recurrence relations are not obtainable for a greatly extended range.

The relationship between the values of a in the two tables is $a_{\text{II}} = a_{\text{I}} + 1$, enabling one to compare the recurrence relation method with the direct one. Thus,

TABLE I

Parabolic Cylinder Function, Derivative and Recurrence Values for $a = -0.4$

	$U(a, x)$			$U'(a, x)$	$U(a+1, x)$	$U(a-1, x)$
X	Present Work	NBS[a]	ERROR			
0.2	0.1024745 (1)	.10261 (1)	0.1320053 (−1)	−0.2101682	0.1076937 (1)	0.3126427
0.4	0.9766767	.97698	0.7098408 (−3)	−0.2788891	0.8355378	0.4742245
0.6	0.9138549	.91382	0.6627721 (−3)	−0.3461711	0.7201462	0.6203275
0.8	0.8394135	.83937	0.2034439 (−3)	−0.3953111	0.5954568	0.7310765
1.0	0.7569056	.75689	0.4055222 (−4)	−0.4268140	0.4836123	0.8052668
1.2	0.6698636	.66986	0.8453784 (−6)	−0.4407156	0.3879738	0.8426337
1.4	0.5817322	.58176	0.4744217 (−5)	−0.4379614	0.3074882	0.8451740
1.6	0.4956561	.49566	0.3487116 (−5)	−0.4205803	0.2405545	0.8171051
1.8	0.4142865	.41429	0.1871308 (−5)	−0.3914187	0.1856085	0.7642765
2.0	0.3396546	.33965	0.8829258 (−6)	−0.3537696	0.1411503	0.6934242
2.2	0.2731192	.27312	0.3865508 (−6)	−0.3110045	0.1057347	0.6114356
2.4	0.2153837	.21538	0.1602274 (−6)	−0.2662587	0.7798217 (−1)	0.5247192
2.6	0.1665685	.16657	0.6324692 (−7)	−0.2221993	0.5660226 (−1)	0.4387384
2.8	0.1263193	.12632	0.2368320 (−7)	−0.1808888	0.4041798 (−1)	0.3577358
3.0	0.9393420 (−1)	.93934 (−1)	0.8285107 (−8)	−0.1437397	0.2838430 (−1)	0.2846410
3.2	0.6849181 (−1)	.68492 (−1)	0.2606587 (−8)	−0.1115467	0.1959842 (−1)	0.2846410

3.4	0.4896661 (−1)	.48967 (−1)	0.6603189 (−9)	−0.8457337 (−1)	0.1330127 (−1)	0.2211336
3.6	0.3432382 (−1)	.34324 (−1)	0.6915728 (−10)	−0.6267003 (−1)	0.8871498 (−2)	0.1678166
3.8	0.2358928 (−1)	.23589 (−1)	0.6779531 (−10)	−0.4540099 (−1)	0.5813597 (−2)	0.9022062 (−1)
4.0	0.1589453 (−1)	.15895 (−1)	0.7237643 (−10)	−0.3216330 (−1)	0.3742473 (−2)	0.6395236 (−1)
4.2	0.1049992 (−1)	.10500 (−1)	0.4982396 (−10)	−0.2228647 (−1)	0.2366290 (−2)	0.4433631 (−1)
4.4	0.6800220 (−2)	.68002 (−2)	0.2931619 (−10)	−0.1510741 (−1)	0.1469297 (−2)	0.3006790 (−1)
4.6	0.4317691 (−2)	.43177 (−2)	0.1584622 (−10)	−0.1002027 (−1)	0.8958306 (−3)	0.1995096 (−1)
4.8	0.2687608 (−2)	.26876 (−2)	0.8103284 (−11)	−0.6503884 (−2)	0.5362478 (−3)	0.1295414 (−1)
5.0	0.1640065 (−2)	.16401 (−2)	0.3978627 (−11)	−0.4131675 (−2)	0.3151240 (−3)	0.8231837 (−2)
6.0	0.1030144 (−3)		0.7577431 (−13)	−0.3107118 (−3)	0.1668540 (−4)	0.6197550 (−3)
7.0	0.3934687 (−5)		0.8839519 (−15)	−0.1382643 (−4)	0.5502266 (−6)	0.2759783 (−4)
8.0	0.9133030 (−7)		0.6765352 (−17)	−0.3664441 (−6)	0.1122916 (−7)	0.7317653 (−6)
9.0	0.1287725 (−8)		0.3425280 (−19)	−0.5808884 (−8)	0.1412097 (−9)	0.1160365 (−7)
10.0	0.1102561 (−10)		0.1141000 (−21)	−0.5523714 (−10)	0.1090802 (−11)	0.1103652 (−9)
11.0	0.5731361 (−13)		0.2479556 (−24)	−0.3157413 (−12)	0.5164163 (−14)	0.6309661 (−12)
12.0	0.1808491 (−15)		0.3485325 (−27)	−0.1086591 (−14)	0.1495811 (−16)	0.2171685 (−14)
13.0	0.3463568 (−18)		0.3144360 (−30)	−0.2253967 (−17)	0.2647260 (−19)	0.4505286 (−17)
14.0	0.4025656 (−21)		0.1808383 (−33)	−0.2820819 (−20)	0.2859587 (−22)	0.5638778 (−20)
15.0	0.2839362 (−24)		0.6591582 (−37)	−0.2131405 (−23)	0.1883783 (−25)	0.4260927 (−23)
16.0	0.1215202 (−27)		0.1513475 (−40)	−0.9729177 (−27)	0.7562776 (−29)	0.1945079 (−26)

[a] Ref. (11). Numbers in parentheses refer to powers of ten.

TABLE II

Parabolic Cylinder Function, Derivative and Recurrence Values for $a = +0.6$

	$U(a, x)$			$U'(a, x)$	$U(a+1, x)$	$U(a-1, x)$
X	Present Work	NBS[a]	ERROR			
0.2	0.1041035 (1)	.10458 (1)	0.1280669 (−2)	−0.9815019	0.7976349	0.1085605 (1)
0.4	0.8706166	.87372	0.3683100 (−2)	−0.7805672	0.5513126	0.9546905
0.6	0.7235714	.72403	0.1056138 (−2)	−0.6905327	0.4304194	0.9076042
0.8	0.5944484	.59437	0.6250144 (−4)	−0.6009693	0.3301727	0.8387487
1.0	0.4828850	.48280	0.1032417 (−3)	−0.5157178	0.2493412	0.7571603
1.2	0.3876907	.38765	0.7276977 (−4)	−0.4374586	0.1862220	0.6700730
1.4	0.3074046	.30739	0.3309961 (−4)	−0.3666450	0.1376926	0.5818282
1.6	0.2405373	.24053	0.1186603 (−4)	−0.3032610	0.1007555	0.4956908
1.8	0.1856086	.18561	0.3273428 (−5)	−0.2472490	0.7291021 (−1)	0.4142967
2.0	0.1411531	.14115	0.4536535 (−6)	−0.1985035	0.5213676 (−1)	0.3396566
2.2	0.1057368	.10574	0.2315392 (−6)	−0.1568084	0.3681629 (−1)	0.2731190
2.4	0.7798338 (−1)	.77984 (−1)	0.2739257 (−6)	−0.1218032	0.2565736 (−1)	0.2153832
2.6	0.5660288 (−1)	.56603 (−1)	0.1843741 (−6)	−0.9298441 (−1)	0.1763697 (−1)	0.1665681
2.8	0.4041827 (−1)	.40418 (−1)	0.1031225 (−6)	−0.6973348 (−1)	0.1195264 (−1)	0.1263191
3.0	0.2838443 (−1)	.28384 (−1)	0.5225178 (−7)	−0.5135743 (−1)	0.7982540 (−2)	0.9393408 (−1)
3.2	0.1959847 (−1)	.19598 (−1)	0.2480942 (−7)	−0.3713419 (−1)	0.5251492 (−2)	0.6849174 (−1)

3.4	0.1330129 (−1)	13301 (−1)	0.1121866 (−7)	−0.2635438 (−1)	0.3401985 (−2)	0.4896658 (−1)
3.6	0.8871506 (−2)	.88715 (−2)	0.4871911 (−8)	−0.1835510 (−1)	0.2169443 (−2)	0.3432381 (−1)
3.8	0.5813600 (−2)	.58136 (−2)	0.2040013 (−8)	−0.1254343 (−1)	0.1361449 (−2)	0.2358927 (−1)
4.0	0.3742474 (−2)	.37425 (−2)	0.8245230 (−9)	−0.8409576 (−2)	0.8405703 −3)	0.1589452 (−1)
4.2	0.2366291 (−2)	.23663 (−2)	0.3211852 (−9)	−0.5530713 (−2)	0.5104574 (−3)	0.1049992 (−1)
4.4	0.1469296 (−2)	.14693 (−2)	0.1200476 (−9)	−0.3567767 (−2)	0.3048316 (−3)	0.6800220 (−2)
4.6	0.8958306 (−3)	.89583 (−3)	0.4267150 (−10)	−0.2257280 (−2)	0.1789725 (−3)	0.4317691 (−2)
4.8	0.5362478 (−3)	.53625 (−3)	0.1417936 (−10)	−0.1400613 (−2)	0.1032896 (−3)	0.2687608 (−2)
5.0	0.3151240 (−3)	.31512 (−3)	0.4246759 (−11)	−0.8522549 (−3)	0.5858627 (−4)	0.1640065 (−2)
6.0	0.1668540 (−4)		0.5076179 (−13)	−0.5295820 (−4)	0.2638167 (−5)	0.1030144 (−3)
7.0	0.5502266 (−6)		0.1183036 (−14)	−0.2008894 (−5)	0.7554584 (−7)	0.3934687 (−5)
8.0	0.1122916 (−7)		0.1095107 (−16)	−0.4641367 (−7)	0.1360941 (−8)	0.9133030 (−7)
9.0	0.1412097 (−9)		0.5861877 (−19)	−0.6522814 (−9)	0.1530710 (−10)	0.1287725 (−8)
10.0	0.1090802 (−11)		0.1933988 (−21)	−0.5571602 (−11)	0.1069004 (−12)	0.1102561 (−10)
11.0	0.5164163 (−14)		0.3966542 (−24)	−0.2891071 (−13)	0.4616512 (−15)	0.5731361 (−13)
12.0	0.1495811 (−16)		0.4983461 (−27)	−0.9110049 (−16)	0.1228954 (−17)	0.1808491 (−15)
13.0	0.2647260 (−19)		0.3686052 (−30)	−0.1742849 (−18)	0.2011796 (−20)	0.3463568 (−18)
14.0	0.2859587 (−22)		0.1444369 (−33)	−0.2023945 (−21)	0.2021237 (−23)	0.4025656 (−21)
15.0	0.1883783 (−25)		0.1749967 (−37)	−0.1426525 (−24)	0.1244396 (−26)	0.2839362 (−24)
16.0	0.7562776 (−29)		0.7404363 (−41)	−0.6101797 (−28)	0.4688726 (−30)	0.1215202 (−27)

[a] Ref. (11). Numbers in parentheses refer to powers of ten.

for example, $U(a+1, x)$ for $a = -0.4$ (column 6 of Table I) should be the same as $U(a, x)$ for $a = 0.6$ (column 2 of Table II). One can see that the agreement improves with increasing x; this is reasonable since the errors in the function and its derivative decrease for increasing x.

TABLE III

Comparison of Approximation Methods with Exact Calculations, $U(-.5, x)$

x	$U(-.5, x)$		
	Exact[a]	Standard Methods[b]	This Work
2.5	0.209611	0.209612	0.209611
2.6	0.184519	0.184520	0.184519
2.7	0.161621	0.161621	0.161621
2.8	0.140858	0.140859	0.140858
2.9	0.122151	0.122151	0.122151
3.0	0.105399	0.105399	0.105399
3.1	0.904914 (−1)	0.904916 (−1)	0.904913 (−1)
3.2	0.773047 (−1)	0.773049 (−1)	0.773047 (−1)
3.3	0.657103 (−1)	0.657104 (−1)	0.657102 (−1)
3.4	0.555762 (−1)	0.555763 (−1)	0.555762 (−1)
3.5	0.467706 (−1)	0.467707 (−1)	0.467706 (−1)
3.6	0.391639 (−1)	0.391640 (−1)	0.391639 (−1)
3.7	0.326308 (−1)	0.326308 (−1)	0.326307 (−1)
3.8	0.270518 (−1)	0.270519 (−1)	0.270518 (−1)
3.9	0.223149 (−1)	0.223150 (−1)	0.223149 (−1)
4.0	0.183156 (−1)	0.183157 (−1)	0.183156 (−1)

[a] From the Hermite polynomials, Eq. (10).
[b] Power series for $x \leqslant 3$; Asymptotic Method otherwise.

One important feature of this method of calculation is its accuracy in the critical range where x is becoming too large for the use of power series and is not large enough for asymptotic methods. Table III shows a comparison of values of $U(a, x)$ calculated by our method with those obtained from power series and the asymptotic method given in Eq. (19.8.1) of Abramowitz and Stegun [8]. It has been our experience that the power series begins to diverge for values of x greater than about 3, and the asympytotic method must be used. We therefore show a range of x from 2.5–4.0 as illustrative of the problem. The value of $a = -0.5$ was chosen because one can calculate $U(a, x)$ exactly via the relationship with the Hermite polynomials, $Hn(x)$. In general, for integral values of n,

$$U(-n - 1/2, x) = 2^{-1/2n} e^{-1/4x^2} H_n(x/\sqrt{2}), \tag{10}$$

and hence the values of $U(-0.5, x)$ shown in the first column of Table III correspond to Eq. (10) with $n = 0$. The values of the parabolic cylinder functions for our method were obtained by use of the recurrence relations. One can see from the table that the new method is at least equal in accuracy, and in some cases superior, compared with the other approximation methods.

In conclusion, this method has been useful in obtaining values of the parabolic cylinder function $U(a, x)$ for a limited range in a and for large values of x, where this method fails, power-series solutions produce accurate results. More accurate results could be obtained for small x, if a larger number of moments could be calculated without overflowing the computer. For larger x values, the use of more moments would lead to less improvement. By using only five moments, the values obtained for large x are very accurate since the error values are extremely small. In fact, the Gaussian quadrature method should produce very accurate values for even larger x values than listed in Tables I and II.

Perhaps the most serious limitation on this method is that it cannot be used for negative values of x. This could be remedied by the use of a similar integral representation for the other linearly independent solution, $V(a, x)$, for then one could use relations [14] of the type

$$\pi V(a, x) = \Gamma[a + (1/2)][U(a, x) \sin \pi a + U(a, -x)]. \tag{11}$$

We are currently exploring this approach.

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