Electronic Transactions on Numerical Analysis.
Volume 9, 1999, pp. 137-146.

ISSN 1068-9613.

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EVALUATION OF ASSOCIATED LEGENDRE FUNCTIONS OFF THE CUT AND PARABOLIC CYLINDER FUNCTIONS*

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Abstract. We review a set of algorithms to evaluate associated Legendre functions off the cut; in particular, we consider prolate spheroidal, oblate spheroidal and toroidal harmonics. A similar scheme can be applied to other families of special functions like Bessel and parabolic cylinder functions; we will describe the corresponding algorithm for the evaluation of parabolic cylinder functions.

Key words. computation of special functions, Legendre functions, parabolic cylinder functions.

AMS subject classifications. 65D20, 33-04, 33C05, 33A70.

1. Introduction.

The evaluation of associated Legendre (ALF) and parabolic cylinder functions (PCF) is a matter of relevance because these functions appear in the solution of Dirichlet problems in different geometries [12]. Then, they show up in a vast number of applications [12, 8, 9] in different fields such as, for instance, lattice field theory[5], thermonuclear fusion[16], biology [10] or cristallography[18].

Recently, a series of codes to evaluate ALF[8, 9, 24] and PCF[23] have been developed, filling a considerable gap in numerical libraries.

For associated Legendre functions off the cut there was no available routine; only Gautschi [6], in 1965, presented a set of algorithms in ALGOL60 to evaluate them. Our approach is similar to Gautschi's: Legendre functions off the cut satisfy three term recurrence relations, being one of the independent solutions a minimal solution [28, 7]. However, our code has some important differences from Gautschi's which, in fact, allows it to be more accurate and valid for a larger range of the parameters [24].

Other examples of families of real functions of real variable satisfying three term recurrences with a minimal solution are Bessel and Modified Bessel functions and parabolic cylinder functions.

Bessel functions have been broadly discussed in the literature and many algorithms with different characteristics exist [19, 2, 27, 26, 22]. But there was a considerable lack of numerical algorithms for PCF: there was only one published program to evaluate PCFs [25], which as we discussed [23], has serious problems. Different approaches to the evaluation of PCFs can be found in [11, 20, 15, 21].

ALFs, PCFs and Bessel functions are classical in the sense that all standard books on special functions [1, 12, 28] devote at least a chapter to them. In addition, the task of developing numerical methods to evaluate the classical special functions has gained renewed interest due to the ongoing program to revise the Abramowitz & Stegun Handbook on Mathematical functions [14]. A comprehensive numerical library to generate values for all functions described in such revised version is intended to be built.

2. Legendre and parabolic cylinder functions: definition and properties.

2.1. Associated Legendre functions off the cut.

The associated Legendre functions $P_\nu^m(z)$ and $Q_\nu^m(z)$ [1] are solutions of the differential equation

*Received November 1, 1998. Accepted for publicaton December 1, 1999. Recommended by F. Marcellán.
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$$(2.1)\qquad (1-z^2)u'' - 2zu' + \left[\nu(\nu+1) - \frac{m^2}{1-z^2}\right]u = 0,$$

where, in most practical situations, m is a nonnegative integer.

From now on we will consider associated Legendre functions with z outside the interval $[-1, 1]$, that is, associated Legendre functions off the cut. For the evaluation of associated Legendre functions on the cut, see [17].

The recurrence relations satisfied by the associated Legendre functions off the cut (ALF), both over degrees ν's and orders m's are

$$(2.2)\qquad (\nu - m + 1)P^m_{\nu+1}(z) - (2\nu+1)zP^m_\nu(z) + (\nu+m)P^m_{\nu-1}(z) = 0,$$

$$(2.3)\qquad P^{m+1}_\nu(z) + \frac{2mz}{(z^2-1)^{1/2}}P^m_\nu(z) - (\nu - m + 1)(\nu+m)P^{m-1}_\nu = 0,$$

where the same relations apply for the Q's.

The Wronskian relation between P's and Q's is

$$(2.4)\qquad W(P^m_\nu(z), Q^m_\nu(z)) = \frac{\Gamma(\nu+m+1)}{\Gamma(\nu-m+1)}\frac{(-1)^m}{1-z^2}.$$

From which follow two useful relations between consecutive degrees (eq.(5)) and orders (eq.(6))

$$(2.5)\qquad P^m_\nu(z)Q^m_{\nu-1}(z) - P^m_{\nu-1}(z)Q^m_\nu(z) = \frac{\Gamma(\nu+m)}{\Gamma(\nu-m+1)}(-1)^m,$$

$$(2.6)\qquad P^m_\nu(z)Q^{m+1}_\nu(z) - P^{m+1}_\nu(z)Q^m_\nu(z) = \frac{\Gamma(\nu+m+1)}{\Gamma(\nu-m+1)}\frac{(-1)^m}{\sqrt{z^2-1}}.$$

For half-integer degrees $\nu \equiv n - 1/2$, $n = 0, 1, 2, ...$ and real arguments $z \equiv x > 1$, the functions $\{P^m_{n-1/2}(x), Q^m_{n-1/2}(x)\}$ are called *toroidal harmonics*. When ν is an integer $\nu \equiv n = 0, 1, 2, ...$ and for real arguments $x > 1$, the functions $\{P^m_n(x), Q^m_n(x)\}$ are called *prolate spheroidal harmonics*, while, for purely imaginary arguments, the functions $\{P^m_n(ix), Q^m_n(ix)\}$ with $x > 0$ are known as *oblate spheroidal harmonics*.

Both prolate spheroidal and toroidal harmonics are real functions of the real variable x. The oblate spheroidal harmonics $\{P^m_n(ix), Q^m_n(ix)\}$ can be real or imaginary valued for real x; however, the new set of functions $\{R^m_n(x), T^m_n(x)\}$ $x > 0, n \geq 0$ defined by

$$(2.7)\qquad \begin{aligned} R^m_n(x) &= exp(-i\frac{\pi n}{2})P^m_n(ix), \\ T^m_n(x) &= iexp(i\frac{\pi n}{2})Q^m_n(ix) \end{aligned}$$

are real functions of the real variable x, and more convenient for numerical evaluation. From now on, we will refer to $R^m_n(x)$ and $T^m_n(x)$ as *oblate spheroidal harmonics* (OSH) of the first and second kinds respectively. Reference [9] is the first one to provide a numerical algorithm to compute OSHs.

2.2. Parabolic cylinder functions. The parabolic cylinder functions $V(a,x)$ and $U(a,x)$ [1] are solutions of the differential equation

$$y'' - (a + \frac{1}{4}x^2)y = 0 \ . \tag{2.8}$$

The Vs and Us satisfy the following recurrence relations:

$$V(a+1,x) = xV(a,x) + (a-1/2)V(a-1,x), \tag{2.9}$$

$$U(a-1,x) = xU(a,x) + (a+1/2)U(a+1,x). \tag{2.10}$$

The Wronskian relation between V's and U's is

$$W\{U(a,x),V(a,x)\} = \sqrt{2/\pi} \tag{2.11}$$

from which it follows that

$$(a-1/2)U(a,x)V(a-1,x) + U(a-1,x)V(a,x) = \sqrt{\frac{2}{\pi}} \ . \tag{2.12}$$

3. Recurrence relations and stability. Both associated Legendre $\{P,Q\}$ and parabolic cylinder functions $\{U,V\}$ have two common characteristics: they satisfy three-term recurrence relations and one of the solutions is minimal.

A three term recurrence relation

$$y_{k+1} + a_k y_k + b_k y_{k-1} = 0 \tag{3.1}$$

is said to admit a minimal solution when there exist two linearly independent solutions $y_k^{\downarrow}$, $y_k^{\uparrow}$ such that

$$\lim_{k\to\infty} \frac{y_k^{\downarrow}}{y_k^{\uparrow}} = 0; \tag{3.2}$$

the solution $y_k^{\downarrow}$ is called minimal solution (which is unique) while $y_k^{\uparrow}$ is a dominant solution. The recurrence relation should be applied backwards to evaluate the minimal solution, and never forward, since any small rounding error would introduce a dominant component. On the other hand, the recurrence relation has to be applied forward to calculate dominant solutions.

Important results are provided by Perron's [28, 19] and Pincherle's[3, 19] theorems: Perron's theorem helps in studying the stability of recurrences and the existence of a minimal solution. On the other hand, Pincherle's theorem guarantees the existence of a continued fraction (CF) for the ratio of consecutive minimal solutions $y_k^{\downarrow}/y_{k-1}^{\downarrow}$ and gives a prescription to estimate the speed of convergence of the resulting CF; in case the recurrence (3.1) admits minimal solution Pincherle's theorem states that the ratio can be evaluated in the form:

$$y_k^{\downarrow}/y_{k-1}^{\downarrow} = -\frac{b_k}{a_k-}\frac{b_{k+1}}{a_{k+1}-}\cdots \tag{3.3}$$

It is easy to check that Q_ν^m is the minimal solution of the three term recurrence relation (2.2) while P_ν^m is a dominant solution. Correspondingly, for oblate spheroidal harmonics, the minimal solution is T_n^m and the dominant one is R_n^m. The character of the functions Q_ν^m, P_ν^m changes if one consider the recurrence relation given by eq.(2.3): P_ν^m is the minimal solution while Q_ν^m is a dominant one. Notice that, in case ν is integer, because $P_n^m = 0$ when $m > n$ and n, m are integers, the CF (3.3) for the ratio P_{n-1}^m/P_n^{m-1} becomes a finite continued fraction.

For prolate and oblate spheroidal harmonics we always assume $n \geq m$; the recurrence over n starting with $n = m$ and $n = m + 1$ will be enough for their evaluation. However, the evaluation of TH, needs both recurrences (over m and n).

In the case of parabolic cylinder functions, one can easily establish the character of U's as the minimal solution of recurrence (2.10) and the character of Vs as a dominant one of (2.9). We have focused our attention on integer and half-integer values of the order a and non-negative arguments x which are the cases of greatest applicability.

4. Numerical evaluation of ALF and PCF.

The numerical evaluation of PSH, OSH and PCF follow a similar scheme and the procedure can be described in terms of a single basic algorithm. The main differences are in the evaluation of the starting values to "feed" the recurrences, the study of the convergence of the continued fraction (and substitution whenever it converges slowly) and the handling of possible numerical overflows. For issues of convergence of the CFs and control of overflows, we refer to [8, 9, 23, 24]. We describe the basic algorithm and the evaluation of the starting values. Also, we will explicitly show the resulting algorithm for OSH.

The algorithms for the evaluation of TH are considerably more involved. In this case, both recurrences have to be combined in the algorithm. We will present one of the three algorithms described in ref. [24]

4.1. Basic algorithm.

The main ingredients of our algorithms are the character of the functions as minimal or dominant solutions of a three term recurrence relation and the Wronskian relating both solutions. Essentially the procedure can be described as follows: Given a three term recurrence relation

$$y_{k+1} + a_k y_k + b_k y_{k-1} = 0, \quad k \geq 1 \tag{4.1}$$

with $y_k^{\downarrow}$ the minimal solution and $y_k^{\uparrow}$ a dominant one, and considering

$$y_k^{\downarrow} y_{k-1}^{\uparrow} + c_k(x) y_{k-1}^{\downarrow} y_k^{\uparrow} = d_k(x) \tag{4.2}$$

the Wronskian relating both solutions, the following steps are considered to evaluate the set $\{y_k^{\uparrow}, y_k^{\downarrow}, k = 0, 1, ...K\}$:

- ◯ Evaluate $y_0^{\uparrow}, y_1^{\uparrow}$.
- ◯ Use forward recurrence to obtain the set $\{y_0^{\uparrow}, y_1^{\uparrow}, ..., y_K^{\uparrow}\}$.
- ◯ Combine $y_K^{\downarrow}/y_{K-1}^{\downarrow} = -\frac{b_K}{a_K-}\frac{b_{K+1}}{a_{K+1}-}\cdots$ with the Wronskian relation (4.2) and $y_K^{\uparrow}, y_{K-1}^{\uparrow}$ to get $y_K^{\downarrow}, y_{K-1}^{\downarrow}$.

◯ Use backward recurrence to obtain $\{y_K^{\downarrow}, y_{K-1}^{\downarrow}, ..., y_0^{\downarrow}\}$.

Some interesting features of the algorithm described are: first, unlike Miller's method, no renormalization has to be carried out. This is important in order to have a good control of accuracy and overflows. Second, both dominant and minimal solutions can be obtained at the same time; this feature is of interest when both solutions are needed, as happens when solving Dirichlet problems.

The basic ingredient in Gautschi's codes for PSH and TH was also the application of recurrence relations. However, although the underlying theory is the same as in Gautschi's codes, our approach leads to algorithms valid for larger ranges of the parameters, much faster when several orders/degrees are needed, and with higher precision [24].

On the other hand, surprisingly, recurrence relations where rarely used for PCF and the associated continued fraction and, useful as it is, was not considered in [11, 20, 15, 21]. Our code for PCFs, as we discussed in [23], solves the problems of Taubmann's code [25] and enlarges considerably the ranges of parameters.

In principle, we only need to evaluate the two starting values for the recurrences. However, one also needs to take care of possible bad convergence of the CFs (taking into account Pincherle's theorem) and to replace the CF by series or asymptotic expansions when needed. For more details see [23, 24].

Let us now summarize how the evaluation of the starting values is carried in each of the cases described.

4.2. Evaluation of the starting values for the recurrences. To feed the recurrence relations we need two starting values, which are evaluated as follows:

◯ Prolate and oblate spheroidal harmonics:

For prolate and oblate spheroidal harmonics a closed expression can be found for the initial values:

$$P_m^m(x) = (2m-1)!!(x^2-1)^{m/2}\ ;\ P_{m+1}^m(x) = x(2m+1)P_m^m(x), \tag{4.3}$$

$$R_m^m(x) = (2m-1)!!(x^2+1)^{m/2}\ ;\ R_{m+1}^m(x) = x(2m+1)R_m^m(x). \tag{4.4}$$

◯ Toroidal harmonics:

In this case we use the relation of $Q^0_{-1/2}$ and $Q^1_{-1/2}$ with the elliptic integrals E and K:

$$\begin{aligned} Q^0_{-1/2}(x) &= \sqrt{2/(x+1)}K(\sqrt{2/(x+1)}), \\ Q^1_{-1/2}(x) &= -E(\sqrt{2/(x+1)})/\sqrt{2(x-1)}, \end{aligned} \tag{4.5}$$

and we evaluate E and K by means of the Carlson's duplication theorem[4].

◯ Parabolic cylinder functions of integer order $a \geq 0$:

For parabolic cylinder functions $V(a,x)$ with integer values of the parameter a, we consider the relation of $V(0,x)$ and $V(1,x)$ with the modified Bessel functions I_ν

$$V(0,x) = \frac{\sqrt{x}}{2}\left(I_{-1/4}(x^2/4) + I_{1/4}(x^2/4)\right) \tag{4.6}$$

$$V(1,x) = \frac{x^{3/2}}{4} \quad \big(I_{-1/4}(x^2/4) + I_{1/4}(x^2/4) + I_{-3/4}(x^2/4) + I_{3/4}(x^2/4)\big)\,. \tag{4.7}$$

To evaluate the Bessel functions we have followed the scheme of reference [19], complemented with an asymptotic expansion [23] for large x.

○ Parabolic cylinder functions of half-integer order $a \geq 1/2$:
In the half-integer case, the expressions for the initial parabolic cylinder functions are simpler:

$$V(1/2,x) = \sqrt{\frac{2}{\pi}} e^{x^2/4}\ ;\ V(3/2,x) = \sqrt{\frac{2}{\pi}} x e^{x^2/4}. \tag{4.8}$$

4.3. An explicit example: oblate spheroidal harmonics. As an example of the basic algorithm, we show the corresponding to the evaluation of oblate spheroidal harmonics:

Let $r_n(x) = R^m_{m+n}(x)$ and $t_n(x) = T^m_{m+n}(x)$. The following steps are followed to evaluate the set $\{r_n, t_n,\, n = 0, ..., N\}$:

○ Evaluate $r_0(x) = (2m-1)!!(x^2+1)^{m/2} > 0$ and $r_1(x) = x(2m+1)r_0(x) \geq 0$.

○ Apply the recurrence relation

$$r_{n+1} = \frac{1}{n+1}[(2n+2m+1)x r_n(x) + (n+2m)r_{n-1}(x)] \geq 0$$

(forward) up to a maximum degree $n = N$.

○ Use the Wronskian relation, combined with the CF for $H_N(x) = t_N(x)/t_{N-1}(x)$ (convergent for $x > 0$) to obtain

$$t_{N-1} = \frac{(2m+N-1)!}{N!}(-1)^m \frac{1}{r_N(x) + H_N(x) r_{N-1}(x)},$$

$$t_N(x) = t_{N-1}(x) H_N(x).$$

○ Using t_N, t_{N-1} as starting values, the recurrence relation

$$t_{n-1}(x) = \frac{1}{(n+2m)}[(n+1)t_{n+1}(x) + (2n+2m+1)x t_n(x)]$$

is applied backwards.

Taking into account that $R^m_n(x) \geq 0$, $T^m_n(x) \geq 0\, \forall x \geq 0$, one can see that no subtractions take place in applying the forward and the backward recurrences for $R^m_n(x)$ and $T^m_n(x)$ respectively. Then, no significant roundoff errors are expected to occur.

4.4. A more involved example: toroidal harmonics.. The algorithm for toroidal harmonics (TH) deserves a separate analysis. The main difficulty, compared with OSH and PSH, concerns the starting point of the algorithm. For TH we do not have closed form expressions like (4.3), (4.4), which allowed the evaluation of OSH and PSH for fixed m using only recurrence (2.2). For TH one needs to use recurrence (2.2) combined with (2.3).

As commented, the Q's are minimal and the P's dominant for recursion over the degree n while, for recursion over the order m, the P's are the minimal solution and the Q's dominant. This "dual" behavior together with the two associated CF's and the two Wronskian relations (2.5) and (2.6) makes it possible to reach any order m or degree n from two starting and consecutive values. Using this fact, the algorithm for toroidal harmonics can be summarized as follows:

The set $\{P^m_{n-1/2}, Q^m_{n-1/2}\}$, $n = 0, 1, ..., N+1$, $m = 0, 1, ..., M$ can be generated from:

a) m-recurrence (basic algorithm):
Starting from $Q^0_{-1/2}$ and $Q^1_{-1/2}$, generate $\{P^m_{-1/2}, Q^m_{-1/2},\ 0 \leq m \leq M\}$
(for large x better use series for $P^M_{-1/2}$ instead of the CF).
b) evaluate $P^M_{+1/2}$ (and $P^{M-1}_{+1/2}$):
$Q^M_{-1/2}, H = Q^M_{+1/2}/Q^M_{-1/2} \rightarrow Q^M_{1/2}$
$Q^M_{-1/2}, Q^M_{1/2}, P^M_{-1/2} \rightarrow P^M_{1/2}$ (from the Wronskian).
c) m-recurrence (backward):
$P^M_{1/2}, P^{M-1}_{1/2} \rightarrow P^m_{1/2}, 0 \leq m \leq M$
Then a)+c) give $P^m_{\pm 1/2}$ with $0 \leq m \leq M$.
d) n-recurrence (forward):
$P^m_{-1/2}, P^m_{+1/2}\ 0 \leq m \leq M \rightarrow P^m_{n-1/2}\ 0 \leq m \leq M, 0 \leq n \leq N.$
e) CF + Wronskian to get $Q^0_{N+1/2}, Q^0_{N-1/2}$ from $P^0_{N+1/2}, P^0_{N-1/2}$.
And similarly we get $Q^1_{N+1/2}, Q^1_{N-1/2}$.
f) m-recurrence (forward):
$Q^0_{N\pm 1/2}, Q^1_{N\pm 1/2} \rightarrow Q^m_{N\pm 1/2}, 0 \leq m \leq M.$
g) n-recurrence (backward):
$Q^m_{N+1/2}, Q^m_{N-1/2}, 0 \leq m \leq M \rightarrow Q^m_{n\pm 1/2}, 0 \leq m \leq M, 0 \leq n \leq N.$

This algorithm for toroidal harmonics evaluates and stores in each run first and second kind toroidal harmonics.

4.5. Numerical tests and CPU times. In all cases, our algorithms have been extensively tested in order to control the accuracy and CPU times [8, 9, 24]. In the case of slow convergence of the CF, we have replaced it with series or asymptotic expansions. For parabolic cylinder functions of integer orders a, we have compared our code with other existing code by Taubmann [25], concluding that our code [23] clearly supersedes it.

In double precision arithmetic, the codes for PSH and OSH were shown to reach an accuracy of 10^{-15} in their ranges of validity. For PCF and TH the accuracy was better than 10^{-12}.

In tables 1, 2, 3 and 4 we show the CPU time spent on a HP715/100 computer for our routines to evaluate prolate spheroidal harmonics (DPROH), oblate spheroidal harmonics (DOBLH), toroidal harmonics (DTORH3) and parabolic cylinder functions of integer orders (DINPCF), respectively.

Routine DOBLH uses the algorithm explicitly shown and DPROH use a similar one. Both routines evaluate, for a fixed order m, the first and second kind corresponding ALF's of orders $n = 0, 1, ..., N$ (with N chosen at will). Routine DINPCF also uses our basic algorithm to evaluate integer order PCF's of the first and second kinds of orders $n = 0, ..., N$. Routine DTORH3 uses the algorithm described in section 4.4.

x	M	N_{Max}	$10^3\times$ CPU-t $N=N_{Max}$	$10^3\times$ CPU-t $N=10$
1.01	5	4393	$10.87s$	$0.27s$
	50	1983	$5.06s$	$0.16s$
1.1	5	1411	$3.51s$	$0.14s$
	50	709	$1.88s$	$0.15s$
10.	5	208	$0.54s$	$0.07s$
	50	92	$0.26s$	$0.12s$
1000.	5	79	$0.20s$	$0.06s$
	50	14	$0.06s$	$0.11s$

Table 1. Subroutine DPROH. CPU times (in 10^{-3} s) for several values of x and M. The demanded precision is EPS=10^{-15}. N_{Max} accounts for the maximum order that can be reached for an overflow 1.d+280.

x	M	N_{Max}	$10^3\times$ CPU-t $N=N_{Max}$	$10^3\times$ CPU-t $N=10$
0.01	5	60803	$153.57s$	$4.11s$
	50	15472	$46.73s$	$4.76s$
0.1	5	6211	$15.48s$	$0.46s$
	50	2651	$6.87s$	$0.50s$
1.	5	712	$1.77s$	$0.10s$
	50	365	$1.00s$	$0.15s$
10.	5	208	$0.51s$	$0.07s$
	50	92	$0.32s$	$0.12s$
1000.	5	79	$0.23s$	$0.06s$
	50	14	$0.13s$	$0.12s$

Table 2. Subroutine DOBLH. CPU times (in 10^{-3} s) for several values of x and M. The demanded precision is EPS=10^{-15}. N_{Max} accounts for the maximum order that can be reached for an overflow 1.d+280.

x	$10^2\times$ CPU-t. M ≤ 50 ; N ≤ 50
1.1	$1.41s$
10.	$1.43s$
100.	$1.41s$
1000.	$1.41s$

Table 3. Subroutine DTORH3. CPU times (in 1/100 s) in evaluating $\{P^m_{n-1/2}, Q^m_{n-1/2}\}$ for several values of x, $m = 0, 1, ..., 50$ and $n = 0, 1, ..., 50$. The demanded precision is EPS=10^{-12}.

x	N_{Max} MODE=0	$10^3\times$CPU-t $N = N_{Max}$	N_{Max} MODE=1	$10^3\times$CPU-t $N = N_{Max}$	$10^3\times$CPU-t $N = 10$
0.1	276	$0.54s$	276	$0.54s$	$0.09s$
1.0	271	$1.63s$	271	$1.67s$	$0.12s$
2.0	265	$0.91s$	265	$0.88s$	$0.28s$
10.	222	$0.46s$	230	$0.48s$	$0.13s$
1000.			93	$0.17s$	$0.06s$

Table 4. Subroutine DINPCF. CPU times (in 10^{-3} s) for several values of x and N. EPS=10^{-15}. N_{Max} accounts for the maximum order that can be reached for an overflow 1.d+280.

5. Conclusions. A set of algorithms to evaluate oblate and prolate spheroidal harmonics, toroidal harmonics and parabolic cylinder functions of integer and half-integer orders, have been described. These functions appear in a large variety of fields. Prolate spheroidal and oblate spheroidal harmonics appear in the solution of the potential problems for domains bounded by spheroids while toroidal harmonics appear in domains bounded by tori. On the other hand, parabolic cylinder functions of integer and half-integer orders are used in statistical thermodynamics, lattice field theory, etc. In spite of their importance, there were very few codes in the numerical libraries to evaluate them. Our algorithms and the resulting codes fill this gap.

Acknowledgments. The authors wish to thank the Departamento de Física Teórica (U. Valencia) the use of their computer facilities. The authors also would like to acknowledge the hospitality of CWI (Amsterdam) where this work was concluded.

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