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ABSTRACT

Associated Legendre functions of half-odd degree and arguments larger than one, also known as toroidal harmonics, appear in the solution of Dirichlet problems with toroidal symmetry. It is shown how the use of series expansions, continued fractions and uniform asymptotic expansions, together with the application of recurrence relations over degrees and orders, permits the evaluation of the whole set of toroidal functions for a wide range of arguments, orders and degrees. In particular, we provide a suitable uniform asymptotic expansion for $P_\nu^m(x)$ (for large m) which fills the gap left by previous methods.

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1. Introduction

Associated Legendre Functions $\{P_\nu^m(z), Q_\nu^m(z)\}$ appear in the solutions in curvilinear coordinates of the boundary value problems of potential theory for certain domains (the sphere, spheroid, torus). These are analytic functions of z in the plane cut along $(-\infty, 1]$ and are solutions of the differential equation

$$(1-z^2)u'' - 2zu' + \left[\nu(\nu+1) - \frac{m^2}{1-z^2}\right] u = 0 \ , \tag{1.1}$$

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

When $z \in (-1,1)$ (on the cut) the functions $\{P_n^m(z), Q_n^m(z)\}$, conveniently redefined (see [15], Eq. (7.12.5)), are called spherical harmonics (SH) when n and m are nonnegative integers; they appear in the solutions of the Dirichlet problem for a sphere. Spherical harmonics are well-known functions for which accurate and extensive methods of evaluation for wide ranges of n (degree) and m (order) have been described see Olver & Smith [19].

Off the cut, Associated Legendre Functions (ALF) are the natural basis to solve the Dirichlet problem for domains bounded by spheroids and tori. In particular, when n and

m are positive integers, $\{P_n^m(x), Q_n^m(x)\}$ for $x > 1$ appear for prolate spheroidal domains, $\{P_n^m(ix), Q_n^m(ix)\}$ for $x > 0$ solve the boundary problem for an oblate spheroid [12] and $\{P_{n-1/2}^m(x), Q_{n-1/2}^m(x)\}$, $x > 1$ are the solutions for a torus. We will refer to these set of functions, respectively, as prolate spheroidal harmonics (PSH), oblate spheroidal harmonics (OSH) and toroidal harmonics (TH).

In particular, toroidal harmonics appear naturally in the solution of Dirichlet problems with boundary conditions on a torus. They appear, for instance, in the expansion of vacuum magnetic fields in stellators and tokamaks [16] (see also [17]) and they also provide analytical solutions of Poisson's equation for realistic shapes of ion channels [14, 13]. Both functions (P, Q) for different orders (m) and degrees (n) and fixed values of x appear when solving Dirichlet problems for a region bounded by a torus.

Contrary to spherical harmonics, there are few references concerning the numerical evaluation of PSH, OSH [12] and TH [21]. Previous to the methods presented in [11, 12, 21], the only codes for the numerical evaluation of ALF off the cut (including PSH and TH) were built by Gautschi in 1965 [9], based on three-term recurrence relations and Miller's algorithm. Fettis (1970) [7] describes a method for TH which is a generalization of Gauss or Landen's transformation for computing elliptic integrals; such method is potentially useful for small values of the argument and fixed n, m.

Recently, Fortran codes to evaluate PSH, OSH [12] and TH [21] were built. By using recurrence relations, combined with the use of continued fractions and Wronskian relations, codes for the evaluation of PSH and OSH whose range of applicability was only limited by the overflow numbers of the machine were developed. On the other hand, the same kind of techniques applied to TH [21] gave rise to codes with a relative accuracy of 10^{-12} for a wide region in the (x, m) plane, but restricted for too large values of m and x. Despite its limitations, the code in ref. [21] improves Gautschi's scheme and clearly outperforms the computations based on series expansions ([13], [16]).

In this paper, we present a uniform asymptotic expansion for $P_\nu^m(x)$ with ν fixed (real and non-integer) and large m ($m \in \mathbb{N}$) which is uniformly valid for large positive x. A method to compute THs can then be given which significantly improves the range of applicability of the code in ref. [21]. In this way, a scheme to compute THs for wide range of integer orders, half-odd degrees and real arguments (larger than one) is provided.

2. Recurrent schemes to evaluate toroidal functions

Both Legendre functions $P_\nu^m(x)$ and $Q_\nu^m(x)$ satisfy the recurrence relations

$$(\nu - m + 1)P_{\nu+1}^m(x) - (2\nu + 1)xP_\nu^m(x) + (\nu + m)P_{\nu-1}^m(x) = 0 \tag{2.1}$$

and

$$P_\nu^{m+1}(x) + \frac{2mx}{(x^2-1)^{1/2}}P_\nu^m(x) - (\nu - m + 1)(\nu + m)P_\nu^{m-1} = 0\ . \tag{2.2}$$

By using Perron's theorem [10, 22] it is seen that both recurrences (Eqs. (2.1) and (2.2)) admit a minimal solution when $x > 1$: for equation (2.1), $Q_\nu^m(x)$ is minimal and $P_\nu^m(x)$ is dominant; for equation (2.2), $P_\nu^m(x)$ is minimal and $Q_\nu^m(x)$ is dominant.

This dual behavior of the P and Q functions with respect to recursion will be fundamental in order to build stable algorithms. Another consequence derived from the existence of minimal solutions is given by Pincherle's theorem ([3, 18]) which guarantees the convergence of the continued fraction for the ratio of consecutive minimal solutions. Thus, the continued fractions given by the iteration of the expressions

$$H_Q(\nu,m,x) := \frac{Q_\nu^m(x)}{Q_{\nu-1}^m(x)} = \frac{1}{\frac{2\nu+1}{\nu+m}x - \frac{\nu-m+1}{\nu+m}\frac{Q_{\nu+1}^m(x)}{Q_\nu^m(x)}}\,, \tag{2.3}$$

and

$$H_P(\nu,m,x) := \frac{P_\nu^m(x)}{P_\nu^{m-1}(x)} = \frac{(\nu-m+1)(\nu+m)}{\frac{2mx}{\sqrt{x^2-1}} + \frac{P_\nu^{m+1}(x)}{P_\nu^m(x)}}\,. \tag{2.4}$$

are convergent for $x > 1$. The CF from Eq. (2.3) is more rapidly convergent as x becomes larger, while the convergence of the CF in Eq. (2.4) is faster as x becomes smaller (but $x > 1$). In other words, the numerical convergence of Eq. (2.3) may fail when x is too close to 1 while Eq. (2.4) converges slowly for large x.

Except for the possible convergence failures of the continued fractions, algorithms for the computation of the set $\{P_{n-1/2}^m(x), Q_{n-1/2}^m(x),\ x > 1,\ n = 0,1,...,N,\ m - 0,1,...,M\}$ can be based on the calculation of two values to "feed" the recurrences, the stable application of the recurrences (Eqs. (2.2),(2.1)) both for the Ps and the Qs, and the application of the Wronskian relations

$$P_\nu^m(x)Q_{\nu-1}^m(x) - P_{\nu-1}^m(x)Q_\nu^m(x) = \frac{\Gamma(\nu+m)}{\Gamma(\nu-m+1)}(-1)^m \tag{2.5}$$

$$P_\nu^m(x)Q_\nu^{m+1}(x) - P_\nu^{m+1}(x)Q_\nu^m(x) = \frac{\Gamma(\nu+m+1)}{\Gamma(\nu-m+1)}\frac{(-1)^m}{\sqrt{x^2-1}} \tag{2.6}$$

A simple example for evaluating such a set is provided by the following scheme (DTORH3 in [21]), which we will call the *primal* algorithm :

A) Evaluate $P_{\pm 1/2}^m$, $m = M, M-1$ by using the following scheme:

1. Obtain the starting values, $Q_{-1/2}^0$ and $Q_{-1/2}^1$ through their relation with elliptic integrals (evaluated by using Carlson's duplication theorem [4, 5]).
2. Apply the recurrence Eq. (2.2) for Q up to the order M.
3. Combine the values of $Q_{-1/2}^M$ and $Q_{-1/2}^{M-1}$ with the Wronskian relation (2.6) and the CF (2.4) to get $P_{-1/2}^M$.
4. Use the CF (2.3) to obtain $Q_{1/2}^M$ from $Q_{-1/2}^M$ and then obtain $P_{1/2}^m$ from Eq. (2.5) and the already calculated values $Q_{\pm 1/2}^m$ and $P_{-1/2}^M$.

B) Evaluate the set $\{P_{n-1/2}^m,\ n = 0,1,...,N,\ m = 0,1,..,M\}$:

1. Obtain $\{P^m_{\pm 1/2},\, m=0,1,,,M\}$ starting from $P^M_{\pm 1/2}$ and $P^{M-1}_{\pm 1/2}$ and applying the recurrence Eq. (2.2) backwards.
2. For each m, use Eq. (2.1) forwards to evaluate $\{P^m_{n-1/2},\, n=0,1,...,N,\, m=0,1,..,M\}$, starting from the already evaluated values $P^m_{\pm 1/2}$.

C) Evaluate the set $\{Q^m_{n-1/2},\, n=0,1,...,N,\, m=0,1,..,M\}$:

1. Obtain $Q^k_{N-1/2}$ and $Q^k_{N-3/2}$, $k=0,1$ from the values $P^k_{N-1/2}$, $Q^k_{N-3/2}$ and using the Wronskian (2.5) and the CF (2.3) for $Q^k_{N-1/2}/Q^k_{N-3/2}$.
2. Generate the set $\{Q^m_{N-1/2},\, m=0,1,...,M\}$ starting from $Q^0_{N-1/2}$ and $Q^1_{N-1/2}$ and applying (forwards) recurrence (2.2).
3. Similarly, generate the set $\{Q^m_{N-3/2},\, m=0,1,...,M\}$ starting from $Q^0_{N-3/2}$ and $Q^1_{N-3/2}$
4. For each $m=0,1,...,M$ and starting from the values $Q^m_{N-1/2}$ and $Q^m_{N-3/2}$ obtain the set $\{Q^m_{n-1/2},\, n=0,1,...,N,\, m=0,1,..,M\}$ by applying (backwards) the recurrence (2.1).

The conflictive point in the algorithm presented lies in the different convergence of the continued fractions for $P^M_{-1/2}/P^{M-1}_{-1/2}$, $Q^M_{1/2}/Q^M_{-1/2}$ and $Q^k_{N-1/2}/Q^k_{N-3/2}$, $k=0,1$. While the first one converges better for small x the latter converges faster for large x. Numerical experiments show that for $x>1.001$ the CFs for the Qs converge reasonably well, while the CF for the Ps starts to find problems for $x>20$. Hence, we have to find an alternative way of obtaining $P^m_{-1/2}$ for large x. We will see how a series expansion and a uniform asymptotic expansion for large m are enough to solve the computational problems at large x.

A dual algorithm can be constructed by following a parallel scheme but with the following translations: change P by Q, the recurrence over n by recurrences over m, and the Wronskian relating consecutive orders (m) by the Wronskian relating consecutive degrees (n). In this way, the starting point would be the values $P^0_{-1/2}$ and $P^0_{+1/2}$, and the forward recurrence (2.1) would be applied together with a CF for $Q^0_{N-1/2}/Q^0_{N-3/2}$ and a Wronskian relation in order to obtain $Q^0_{N-1/2}$, and so on. In this case, the four CFs that would come into play are $Q^0_{N-1/2}/Q^0_{N-3/2}$, $P^1_{N-1/2}/P^0_{N-1/2}$, $P^1_{k-1/2}/P^0_{k-1/2}$, $k=0,1$.

The duality between P and Q functions becomes manifest by considering Eqs. (8.2.7) and (8.2.8) in [1]. For the particular case of integer orders and half-odd degrees, we can combine (8.2.8) with (8.2.1) and (8.2.3) to obtain the following relation:

$$Q^m_{n-1/2}(\lambda) = (-1)^n \frac{\pi^{3/2}}{\sqrt{2}\Gamma(n-m+1/2)} (x^2-1)^{1/4} P^n_{m-1/2}(x) \tag{2.7}$$

where $\lambda = x/\sqrt{x^2-1}$. From this and Eqs. (2.3) and (2.4), we observe that $H_Q(n-1/2,m,\lambda) = (m-n+1/2)H_P(m-1/2,n,x)$; then, the rate of convergence of the continued fractions appearing in the two algorithms (primal and dual) can be related. In particular, the continued fractions for the Qs used in the primal algorithm will converge with equal speed as the CFs for the Ps in the dual algorithm when $x = \lambda$, that is, when $x = \sqrt{2}$. On the other hand, the convergence of the Q-continued fraction is faster than the convergence of the P-continued fraction when $x > \sqrt{2}$ and vice-versa. For this reason, we use the primal algorithm when $x \geq \sqrt{2}$ and the dual one when $1 < x < \sqrt{2}$.

From now on, we are only considering the primal algorithm, taking $x \geq \sqrt{2}$. All the discussions that follow will have their counterpart for the dual algorithm when $1 < x < \sqrt{2}$, given Eq. (2.7).

For $x \geq \sqrt{2}$ the Q-continued fractions converge fast; however, the continued fraction $P_{-1/2}^{M-1}/P_{-1/2}^{M-1}$ becomes very slow when x becomes large. Therefore, we need to replace this continued fraction by other types of approximation: we will directly evaluate $P_{-1/2}^{M}$ by some expansion (power series, uniform asymptotic expansion). The steps 3 in **A)** for the primal algorithm will then be replaced by direct computation when x is too large. For the dual algorithm the same kind of change will be needed when x is too close to 1: $Q_{N-1/2}^{0}$ would be given by direct computation which, by considering Eq. (2.7), directly follows from the approximations we will discuss for $P_{-1/2}^{M}$.

In [21] (Eq. (13)) a series expansion for $P_{-1/2}^{M}(x)$ in powers of $1/x^2$ was used in the region $x > 5$ and $x/M > 0.22$ in order to compute toroidal functions with an accuracy better than 10^{-12}. The series was seen to give place to large roundoff errors when M became too large, as could be expected given the fact that the Ps are minimal with respect to the orders (Eq. (2.2)). This is why the series gives limited accuracy within limited regions. It becomes evident at this stage that an expansion for large M and uniformly valid for x is needed in order to improve the range of applicability of the method.

3. Uniform asymptotic expansion for $P_\nu^m(x)$, m large

In this section, we discuss a uniform asymptotic expansion for large m of $P_\nu^m(x)$, $x > 1$, which can also be applied for large arguments x. From Eq. (2.7) follows that this expansion will also provide an asymptotic expansion for $Q_{n-1/2}^m(x)$ for large n which will be valid for x close to 1 (to be used in the dual algorithm).

The recent literature on Legendre functions gives several examples of so-called uniform expansions, in which more than one real or complex parameter plays a role in the asymptotics. We discuss a few aspects of these contributions.

In Dunster [6] an expansion is given for large values of m of the conical functions $P_\nu^m(z)$ with $\nu = -\frac{1}{2} + i\tau$, with $\tau \in [0, Bm]$, where B is an arbitrary positive constant. The expansion is in terms of the modified $K-$Bessel function, and is valid in unbounded $z-$domains. It is obtained by using the differential equation of the Legendre functions. In our case we need fixed values of ν, in particular $\nu = -\frac{1}{2}$, and Dunster's expansion can be used for fixed ν; it is also possible to take $\tau = 0$. However, it will be difficult to obtain the coefficients of the expansion, even for the case $\tau = 0$, and therefore we prefer a method described later in this section.

By using the relation (2.7) it follows that the asymptotic problem can be formulated as follows: to obtain an expansion of $Q_\nu^m(x)$ for large values of ν that holds for fixed m (in particular for $m = 0$), uniformly with respect to z in an interval $(1, x_0)$ where $x_0 > 1$ is a constant.

More general expansions for this problem are obtained by Olver [20], Boyd and Dunster [2] (by using the differential equation), Ursell [23] and Frenzen [8] by using integrals. Boyd and Dunster generalized Olver's result by accepting non-fixed $m-$values. In our approach we use an integral for $P_\nu^m(z)$, which is quite different from the one used by Ursell and Frenzen. Our integral follows from the representation in terms of the Gauss hypergeometric function, and our method can in fact be used for other Gauss functions. As in Ursell's paper, we use an integration by parts procedure to find the coefficients, and the expansion contains only two $K-$Bessel functions. Frenzen's expansion contains an infinite series of $K-$Bessel functions.

For all mentioned results, the coefficients of the expansions are complicated expressions. Olver and Boyd & Dunster give recursion relations for the coefficients, and Ursell and Frenzen also give relations for computing the coefficients. For the numerical algorithm straightforward use of the coefficients determined in this way is not possible, because we need the coefficients for large values of z (when considering $P_\nu^m(z)$) or values of z near 1^+ (when considering $Q_\nu^m(z)$), and for stable computations all coefficients need to be expanded in terms of a certain small parameter.

For our numerical algorithm we derive an expansion that shares several features of the available expansions mentioned above, and that is quite suitable for implementation. We give a few steps in the derivation of the expansion. We verify the accuracy and usefulness by giving several numerical illustrations.

The starting point for our asymptotic expansion is the relation of $P_\nu^{-m}(z)$, which for integer m is directly related to $P_\nu^m(z)$ ([1], Eq. (8.2.5)), with hypergeometric functions ([1], Eq. (8.1.2))

$$P_\nu^{-m}(z) = \frac{1}{\Gamma(m+1)}\left(\frac{z-1}{z+1}\right)^{m/2} F(-\nu,\nu+1,m+1,-\xi)\ , \tag{3.1}$$

where $\xi=(z-1)/2$, together with the integral representation for the hypergeometric function ([1], Eq. (15.3.1)):

$$F(-\nu,\nu+1,m+1,-\xi) = \frac{\Gamma(1+m)}{\Gamma(1+\nu)\Gamma(m-\nu)} I_\xi\ , \tag{3.2}$$

being

$$I_\xi := \int_0^1 t^\nu (1-t)^{m-\nu-1}(1+\xi t)^\nu dt = \xi^\nu I_0(m,\alpha)\ . \tag{3.3}$$

With the change of variable $1-t=e^{-u}$ we obtain

$$I_0(m,\alpha) = \int_0^\infty e^{-mu} u^\nu (u+\alpha)^\nu f_0(u) du\ , \tag{3.4}$$

where

$$\alpha = \ln\left(\frac{z+1}{z-1}\right)\ ,\quad f_0(u) = \left(\frac{1-e^{-u}}{u}\frac{e^{u+\alpha}-1}{u+\alpha}\right)^\nu\ . \tag{3.5}$$

The complication for applying standard methods from asymptotics for large m is the singularity at $u=-\alpha$, in particular if $\alpha\to 0$, that is, $z\to\infty$. Watson's lemma (see Olver [20]) can not be applied in this case. To obtain an expansion in terms of K-Bessel functions, we use an expansion of $f_0(u)$ that is based on values of f_0 and its derivatives at $u = 0$ and $u = -\alpha$, by writing $f_0(u) = a_0 + b_0 u + u(u+\alpha)g_0(u)$. Then we obtain

$$I_0(m,\alpha) = a_0\Phi(\alpha,\nu) + b_0\Psi(\alpha,\nu) + \frac{1}{m}I_1(\alpha,\nu) \tag{3.6}$$

with

$$\begin{aligned} \Phi(\alpha,\nu) &= N(\nu,m,\alpha)K_{\nu+1/2}(m\alpha/2)\ , \\ \Psi(\alpha,\nu) &= -\tfrac{\alpha}{2}N(\nu,m,\alpha)\left(K_{\nu+1/2}(m\alpha/2) - K_{\nu+3/2}(m\alpha/2)\right)\ , \end{aligned} \tag{3.7}$$

being $N(\nu,m,\alpha) = \pi^{-1/2}(\alpha/m)^{\nu+1/2}\Gamma(\nu+1)e^{m\alpha/2}$.

Integration by parts is used to obtain the integral I_1:

$$I_1(m,\alpha) = \int_0^\infty e^{-mu}u^\nu(u+\alpha)^\nu f_1(u)du\ , \tag{3.8}$$

$f_1(u)$ being given by

$$f_1(u) = u(u+\alpha)g_0'(u) + (\nu+1)(2u+\alpha)g_0(u)\ . \tag{3.9}$$

Notice that the integral I_1 has the same structure as I_0 and the procedure can be repeated by writing $f_1(u) = a_1 + b_1 u + u(u+\alpha)g_1(u)$, and so on. We get:

$$I_0(m,\alpha) \sim \Phi(\alpha,\nu)\sum_{k=0}^\infty \frac{a_k}{m^k} + \Psi(\alpha,\nu)\sum_{k=0}^\infty \frac{b_k}{m^k}\ , \tag{3.10}$$

as $m \to \infty$, uniformly with respect to small values of α. The coefficients a_k,b_k are functions of α, and are analytic at $\alpha = 0$.

In the Appendix, we will show that $b_{2k} = 0$, $b_{2k+1} = 2a_{2k+1}/\alpha$, which allows us to write:

$$I_0(m,\alpha) \sim (\alpha/m)^{\nu+1/2}\frac{\Gamma(\nu+1)}{\sqrt{\pi}}e^{m\alpha/2}\sum_{l=0}^1 K_{\nu+l+1/2}(m\alpha/2)\sum_{k=0}^\infty \frac{a_{2k+l}}{m^{2k+l}}\ . \tag{3.11}$$

In particular, for P_ν^m with m a positive integer we get:

$$P_\nu^m(z) \sim (-1)^{m+1}\frac{\sin\nu\pi\Gamma(\nu+m+1)}{\pi^{3/2}}\xi^\nu\sum_{l=0}^1 K_{\nu+l+1/2}(m\alpha/2)\sum_{k=0}^\infty \frac{a_{2k+l}}{m^{2k+l}}\ , \tag{3.12}$$

with $\xi = (z-1)/2$, $\alpha = \ln[(z+1)/(z-1)]$ and the coefficients a_k as given in the Appendix.

The expansions derived in this section are related with the one given in [20], page 465, Eq. (12.13). This follows from a few relations between the Legendre functions. Olver's result is supplied with an error bound for the remainder in the expansion. The error bound (and a bound for the quantity δ_{2p+1} in Olver's expansion, which is not present in our expansion) can be computed by using the coefficients a_k, and the algorithms for these coefficients given in the Appendix. In this paper we have verified the accuracy by using numerical verification of computed function values; see the next section.

4. Computational aspects

In our algorithm, the accurate calculation of $P^m_{-1/2}$ is a key ingredient in the evaluation of toroidal functions for wide ranges of the parameters. We are focusing on the primal algorithm (for $x \geq \sqrt{2}$) given that the numerical discussion that follows has its counterpart for $x < \sqrt{2}$ by considering the dual algorithm.

In order to test the different approximations for the evaluation of $P^m_{-1/2}$ we combined the Fortran code presented in [21], which used a combination of CF and series, with the asymptotic expansion (3.12). The resulting program was coded in double precision arithmetics.

We have performed a numerical study of the different strategies used in the evaluation of $P^m_{-1/2}(x)$, namely: (1) recurrence relation + continued fraction; (2) series; (3) asymptotic expansion. We have studied which are the overlapping regions of validity for the different strategies for a relative accuracy of 10^{-12} (as in [21]). This accuracy proves to be reachable even when high orders and degrees are needed and then, consequently, the recurrence relations have to be applied many times. It is important to keep in mind that the recurrences are always used in their stable direction. Higher precision arithmetic should be considered for wider ranges of the parameters to improve the performance of the CF (2.4), which fails to give results with a precision better than 10^{-12} for moderately large m and/or x. Also, extended arithmetic should be taken into account (as in [19]) in order to avoid overflows. In order to minimize the overflow problems, we have considered the evaluation of the functions (as in [21] for modes 1,2):

$$p_{m,n}(x) := P^m_{n-1/2}(x)/\Gamma(m+1/2) \ ; \ q_{m,n}(x) := Q^m_{n-1/2}(x)/\Gamma(m+1/2) \tag{4.1}$$

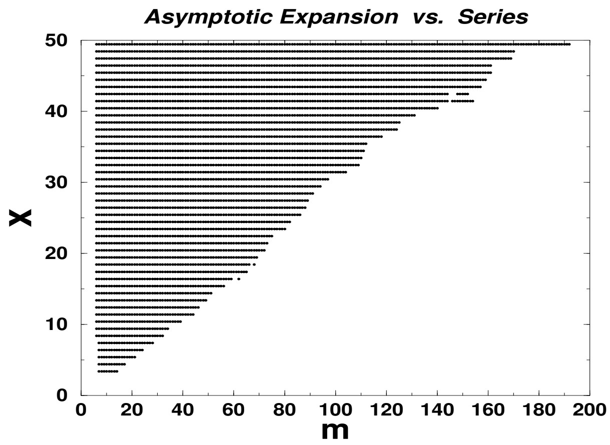

Figure 1. Points in the (m, x)-plane ($m > 0$ integer, $x > 1$) where the numerical values of the toroidal function $P^m_{-1/2}(x)$ obtained by two different methods coincide (values are tested at each increment $\Delta x = 1$). The asymptotic expansion is compared with series expansion for a 12 digits precision. The asymptotic expansion is evaluated up to order m^{-12}; each of the 12 coefficients is expanded up to order α^9.

In Figure 1 we show the comparison between the evaluation of $p_{m,0}$ using the asymptotic expansion and the series. The asymptotic expansion is evaluated up to order m^{-12} and each of the 12 coefficients is expanded up to order α^9. Later we will see that for practical purposes 4 coefficients expanded up to order α^5 are enough. We have plotted the points where both approaches coincide up to a precision better than 10^{-12} in the (m, x) plane. As one can observe, the comparison fails for $x < 4$ (due to the bad convergence of the asymptotic expansion) and for $x/m \lesssim 0.3$ (in this case, due to the series).

In Figure 2 the comparison between the series and the recurrence + continued fraction is shown. In this case, as before, the comparison fails for $x/m \lesssim 0.3$ due to the series. The comparison is also worse as x grows given that the continued fraction starts to converge slowly.

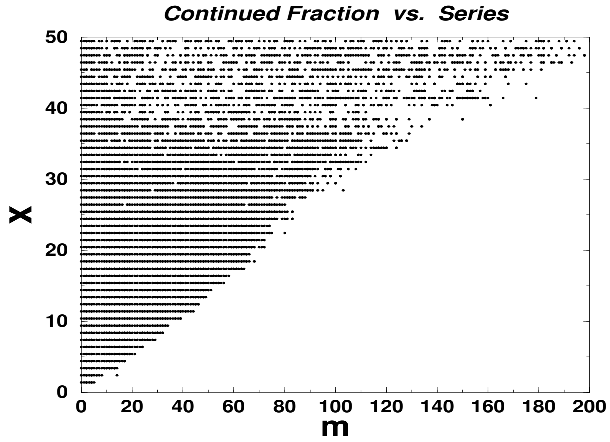

Figure 2. Same as Figure 1, but for other methods of evaluation: the series expansion is compared with the continued fraction method.

Finally, in Figure 3 we compare the computation of $p_{m,0}$ using asymptotic expansion and recurrence + continued fraction. As can be seen in the figure, the comparison fails for $x < 4$ and $m < 6$ (due to the asymptotic expansion) and in the case x is large (due to the continued fraction).

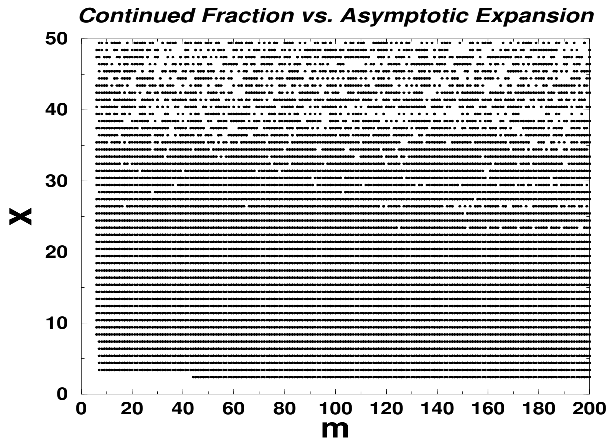

Figure 3. Same as Figure 1, but for other methods of evaluation: the asymptotic expansion is compared with the continued fraction method.

From Figures 1,2 and 3, we conclude that a possible strategy for the evaluation of $p_{m,0}(x)$, for any $x \geq \sqrt{2}$ (primal algorithm) can be the following:

1. Use the CF method (step **A** in the primal algorithm) for moderate x ($x \lesssim 20$).
2. Evaluate $p_{m,0}(x)$ using the series expansion for larger x (typically $x > 5$) but for small $m/x \lesssim 3$
3. Use the asymptotic expansion when the two previous approaches can not be used

In the overlapping regions of validity of the different approximations, the selection of the method of evaluation would depend on the speed of the different methods.

It is worth stressing again that the performance of the continued fractions puts a limit on the attainable accuracy when large ranges of m and n are considered. The limitation of the CF (2.4) was apparent in Figures 2 and 3. Besides, one can also expect that the CF (2.3) will cause a certain loss of accuracy when x is small (in the dual algorithm). However, for the primal algorithm ($x \geq \sqrt{2}$), the convergence of the CF (2.3) is fast and then no further accumulated errors are expected apart from those for CF (Fig. 3). Conversely, the limitation in the dual algorithm comes for the performance of the CF (2.3) and, as for the primal one, with the use of the asymptotic expansion the evaluation in the range $0 \leq m \leq 450$, $0 \leq n \leq 450$ can be performed with a precision of 10^{-12}. In this study, the ranges of m and n are limited by the overflow numbers; notice that the range $0 \leq m \leq 450$ can be reached when $n = 0$ but the range becomes more limited as n increases (see [21] for more details on the available ranges for an overflow number of $\sim 10^{300}$).

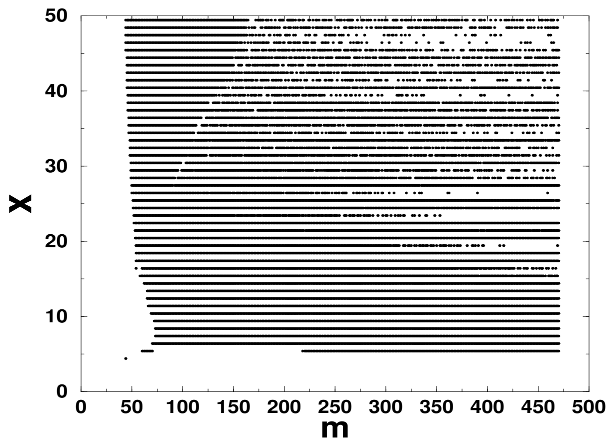

Figure 4. Same as Figure 1, but for other methods of evaluation: the method described in ref. [21] (combining series expansions with the continued fraction method) is compared with the asymptotic expansion with 4 coefficients (given in the Appendix).

In Figure 4 we compare the evaluation of $p_{m,0}(x)$ by using series for $x > 5$ and $x/m > 0.3$ and recurrence relation + CF for the rest of the (m, x)-plane, with the evaluation of $p_{m,0}(x)$ by the asymptotic expansion (using the 4 coefficients explicitly shown at the end of the Appendix). We observe that for a precision of 10^{-12} the asymptotic expansion with 4 coefficients is able to cover the area were the CF is not able to reach the necessary precision. This area was not accurately computable using series or CFs, as discussed in ref. [21]. We then observe that the uniform asymptotic expansion can substitute the use of series or the CF when they fail, namely $x/m \leq 0.3$ and $x > 15$. Furthermore, it can be used in the whole region $x \geq 7$, $m \geq 80$. As shown before, as more coefficients and more terms in the expansion of these coefficients are considered, the asymptotic expansion can be applied for smaller orders and arguments. The number of the coefficients and the number of terms for each coefficient selected for an specific implementation of the method will depend on the timing of the different approaches (series, CF, asymptotic expansion) in the overlapping regions of validity.

5. Conclusions

We have presented a scheme to compute toroidal harmonics for wide ranges of the parameters. By complementing the method presented in [21] with a uniform asymptotic expansion for $P^m_{n-1/2}(x)$ valid for large m and uniformly valid for large x, the toroidal functions can be evaluated with an accuracy of 10^{-12} for $x \geq \sqrt{2}$ in the full range of orders and degrees reachable for an overflow number of $\sim 10^{300}$. Similarly, we discussed how a dual algorithm can be built which, by considering the connection (2.7) between $P^m_{n-1}(x)$ and $Q^n_{m-1/2}$, will also give toroidal functions for $1 < x < \sqrt{2}$ with a precision of at least 10^{-12} for all the orders and degrees reachable within overflow limits.

In this way, an extensive method of computation of toroidal harmonics can be built.

Appendix: Explicit asymptotic formulae

In this appendix we give an explicit algorithm to find the coefficients a_k in the expansions (3.11) (3.12). Previous to this, we will show that the coefficients a_k and b_k in Eq. (3.10) satisfy the relations

$$b_{2k} = 0\ ,\quad b_{2k+1} = 2a_{2k+1}/\alpha \tag{5.1}$$

As explained when we derived expansion (3.10), the coefficients a_k, b_k could be obtained by considering that for $i = 0, 1, ..$

$$\begin{aligned} &f_i(u) = a_i + b_i u + u(u+\alpha)g_i(u)\ ,\\ &f_{i+1}(u) = u(u+\alpha)g_i'(u) + (\nu+1)(2u+\alpha)g_i(u)\ ,\\ &a_i = f_i(0)\ ;\ b_i = (f_i(0) - f_i(-\alpha))/\alpha\ . \end{aligned} \tag{5.2}$$

However, we give now a strategy which is best suited for automatic computation using a symbolic mathematical software package. This algorithm also allows us to prove Eq. (5.1) with ease.

Let us write $f_i(u)$ in the form:

$$f_i(u) = \sum_{k=0}^{\infty} c_k^{(i)} u^k (u+\alpha)^k + u \sum_{k=0}^{\infty} d_k^{(i)} u^k (u+\alpha)^k\ . \tag{5.3}$$

from which follows that $a_i = c_0^{(i)}$, $b_i = d_0^{(i)}$. Let us assume we know the coefficients $c_k^{(0)}, d_k^{(0)}$ for $f_0(u)$. Then the coefficients for $f_i(u), i \geq 1$, can be obtained by recursion, because using the first two equations in (5.2) and a straightforward calculation, we can obtain the following relations

$$
\begin{aligned}
c_0^{(i+1)} &= (\nu+1)\alpha c_1^{(i)} \ , \\
c_k^{(i+1)} &= \alpha[k+\nu+1]c_{k+1}^{(i)} + [2k+2\nu+1]d_k^{(i)} \ , \ \ k=1,2,\dots \ , \\
d_k^{(i+1)} &= 2[k+\nu+1]c_{k+1}^{(i)} - \alpha[k+\nu+1]d_{k+1}^{(i)} \ , \ \ k=0,1,2,\dots \ ,
\end{aligned}
\tag{5.4}
$$

where $i = 0, 1, \ldots$.

Eqs. (5.4) can be applied reiteratively to obtain $a_i = c_0^{(i)}$ and $b_i = d_0^{(i)}$, $i = 0, 1, ..$ starting from the coefficients $c_k^{(0)}$ and $d_k^{(0)}$ which can be automatically generated by using the following scheme.

Consider Eq. (5.3) for $i = 0$ and write $u = w - \alpha/2$, then:

$$
f_0(u(w)) = \sum_{k=0}^{\infty} c_k^{(0)} (w^2 - \alpha^2/2)^k + (w - \alpha/2) \sum_{k=0}^{\infty} d_k^{(0)} (w^2 - \alpha^2/2)^k \ , \tag{5.5}
$$

which gives pure power series by writing

$$
w = \sqrt{v + \alpha^2/4} \ . \tag{5.6}
$$

Then, defining

$$
\begin{aligned}
h_1(v) &:= (f_0(w - \alpha/2) - f_0(-w - \alpha/2))/2w \ , \\
h_2(v) &:= ((w + \alpha/2) f_0(w - \alpha/2) + (w - \alpha/2) f_0(-w - \alpha/2))/2w \ ,
\end{aligned}
\tag{5.7}
$$

we have

$$
h_1(v) := \sum_{k=0}^{\infty} d_k^{(0)} v^k \ , \ \ h_2(v) := \sum_{k=0}^{\infty} c_k^{(0)} v^k \ , \tag{5.8}
$$

and the first set of coefficients $c_k^{(0)}$, $b_k^{(0)}$ can be obtained as Taylor coefficients. In particular, for our definition of f_0 (Eq. (3.5)), we have

$$
\begin{aligned}
& h_1(v) = 0 \Rightarrow d_k^{(0)} = 0 \ , \ \ k = 0, 1, \dots \ , \\
& h_2(v) := e^{\alpha\nu/2} g(v)^\nu \ , \ \ g(v) = \tfrac{2}{v}(\cosh\sqrt{v + (\alpha/2)^2} - \cosh(\alpha/2)) \ .
\end{aligned}
\tag{5.9}
$$

In this way, the coefficients $c_k^{(0)}$ are the Taylor coefficients of the expansion of $h_2(v)$ in powers of v, while we have shown that $d_k^{(0)} = 0$. From these last conditions, it is straightforward to check that

$$
d_k^{(2i)} = 0 \ ; \ \ c_k^{(2i+1)} = \frac{\alpha}{2} d_k^{(2i+1)} \ , \ \ i, k = 0, 1, \dots \ , \tag{5.10}
$$

and thus that relations (5.1) hold.

Then, the generation of the coefficients a_k can be summarized as follows: compute the Taylor coefficients $c_k^{(0)}$ for the expansion of $h_2(v)$ (Eq. 5.9) in powers of v; apply then the recurrences (5.4) to obtain the coefficients $a_i = c_0^{(i)}$.

A more explicit algorithm follows by observing that the Taylor coefficients in the expansion of $g(v)$ (Eq. (5.9)) are related to the modified Bessel functions $I_{k+1/2}(\alpha/2)$. With this interpretation (see also [1], Eq. (10.2.30) and Frenzen's approach in [8]), the evaluation of the coefficients a_i can be summarized as follows:

1. Obtain the coefficients $h_k^{(0)}$:
   (a) Generate the coefficients $\lambda_n = \frac{1}{(n+1)!\alpha^n}\frac{I_{n+1/2}(\alpha/2)}{I_{1/2}(\alpha/2)}$ by symbolic recursion.
   (b) Starting from $h_0^{(0)} = 1$ and $h_1^{(0)} = \nu\lambda_1$ evaluate the coefficients $h_k^{(0)}$ by using:
$$h_{n+1}^{(0)} = \nu\lambda_{n+1} + \frac{1}{n+1}\sum_{j=1}^{n}(n-j+1)[\nu\lambda_{n-j+1}h_j^{(0)} - \lambda_j h_{n-j+1}^{(0)}] \,.$$
2. Obtain the coefficients $a_j = h_0^{(j)}a_0$, where $a_0 = \left(\frac{e^\alpha - 1}{\alpha}\right)^\nu$, through the recurrence
$$h_k^{(i+1)} = \alpha[k+\nu+1]h_{k+1}^{(i)} + (1-(-1)^i)\frac{2}{\alpha}[2k+2\nu+1]h_k^{(i)} \,. \tag{5.11}$$

After evaluating the exact coefficients one should expand them in powers of α in order to avoid roundoff errors as $\alpha \to 0$. As an example, we now give the first 3 coefficients which we used in the section "Computational aspects" (for $\nu = -1/2$):

$$\begin{aligned}
a_0 &= \sqrt{\alpha/(e^\alpha - 1)}\\
h_1^{(0)} &= a_1/a_0 = -\tfrac{1}{48}\alpha + \tfrac{1}{2880}\alpha^3 - \tfrac{1}{120960}\alpha^5 + \ldots\\
h_2^{(0)} &= a_2/a_0 = \tfrac{7}{7680}\alpha^2 - \tfrac{13}{322560}\alpha^4 + \ldots\\
h_3^{(0)} &= a_3/a_0 = \tfrac{7}{1920}\alpha - \tfrac{571}{2580480}\alpha^3 + \ldots
\end{aligned} \tag{5.12}$$

where series expansions in powers of α must also be considered for the computation of a_0 in order to avoid roundoff errors for small α.

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