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1988 J. Phys. A: Math. Gen. 21 3685

(http://iopscience.iop.org/0305-4470/21/19/008)

J. Phys. A: Math. Gen. **22** (1989) 5303. Printed in the UK

ADDENDUM

Computation of eigenvalues of spheroidal harmonics using relaxation Caldwell J 1988 *J. Phys. A: Math. Gen.* **21** 3685-93

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0305-4470/89/245303+01$02.50

J. Phys. A: Math. Gen. 21 (1988) 3685-3693. Printed in the UK

Computation of eigenvalues of spheroidal harmonics using relaxation

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Received 8 December 1987, in final form 8 June 1988

Abstract. Spheroidal harmonics $H_{mn}(x; c)$, where c is the oblateness parameter, arise in the solution of certain partial differential equations by separation of variables in spheroidal coordinates. A numerical method is described which uses relaxation to compute eigenvalues λ_{mn} of $H_{mn}(x; c)$ for the case $m \geq 0$ and $n \geq m$. Such a method is useful if eigenvalues λ_{mn} are required for a large sequence of values of c. The method converges quickly and gives good agreement with exact results.

1. Spheroidal harmonics

Spheroidal harmonics typically arise when certain partial differential equations are solved by the method of separation of variables using spheroidal coordinates. They satisfy the differential equation

$$(1-x^2)\frac{\mathrm{d}^2H}{\mathrm{d}x^2} - 2x\frac{\mathrm{d}H}{\mathrm{d}x} + \left(\lambda - c^2x^2 - \frac{m^2}{1-x^2}\right)H = 0 \tag{1}$$

on the interval $-1 \leq x \leq 1$. Here m is an integer, c is the oblateness parameter and λ is the eigenvalue. Despite the notation, c^2 may be positive or negative. For $c^2 > 0$ the functions are called 'prolate', while if $c^2 < 0$ they are called 'oblate'. The equation has singular points at $x = \pm 1$ and we are interested in the solution with boundary conditions such that the solution is regular at $x = \pm 1$. This will only be possible for certain values of the eigenvalue λ.

The spherical case (where $c = 0$) produces the differential equation for Legendre functions $P_n^m(x)$. In this case the eigenvalues are

$$\lambda_{mn} = n(n+1) \qquad n = m, m+1, \ldots .$$

The integer n labels successive eigenvalues for fixed m. When $n = m$ we have the lowest eigenvalue and the corresponding eigenfunction has no nodes in the interval $-1 < x < 1$. When $n = m+1$ we have the next eigenvalue and the eigenfunction has one node inside $(-1, 1)$, and so on.

A similar situation holds for the general case $c^2 \neq 0$. Writing the eigenvalues of equation (1) as $\lambda_{mn}(c)$ and the eigenvectors as $H_{mn}(x; c)$, then for fixed m, $n = m$, $m+1, \ldots$, labels the successive eigenvalues.

It is important to note that the computation of $\lambda_{mn}(c)$ and $H_{mn}(x; c)$ traditionally has been quite difficult. Relevant complicated recurrence relations, power series expansions, etc, can be found in Abramowitz and Stegun (1968), Flammer (1957) and

Morse and Feshbach (1953). However, low-cost computing makes evaluation by direct solution of the differential equation quite feasible.

The first step is to investigate the behaviour of the solution near the singular points $x = \pm 1$. On substituting a power series expansion of the form

$$H = (1 \pm x)^{\alpha} \sum_{k=0}^{\infty} c_n (1 \pm x)^k \tag{2}$$

into equation (1), we find that the regular solution has $\alpha = m/2$. Without loss of generality we can take $m \geqslant 0$ since $m \to -m$ is a symmetry of the equation. It is preferable to factor out this behaviour and accordingly we set

$$H = (1 - x^2)^{m/2} y \tag{3}$$

We then find from equation (1) that y satisfies the equation

$$(1 - x^2)\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} - 2(m+1)x\frac{\mathrm{d}y}{\mathrm{d}x} + (\mu - c^2 x^2)y = 0 \tag{4}$$

where

$$\mu \equiv \lambda - m(m+1). \tag{5}$$

Both equations (1) and (5) are invariant under the replacement $x \to -x$. Hence the functions H and y must also be invariant, except possibly for an overall scale factor. Since the equations are linear, a constant multiple of a solution is also a solution. Also, since the solutions will be normalised, the scale factor can only be ± 1. If $n - m$ is odd, there are an odd number of zeros in the interval $(-1, 1)$. Thus we must choose the antisymmetric solution $y(-x) = -y(x)$ which has a zero at $x = 0$. Conversely, if $n - m$ is even we must have the symmetric solution. Thus

$$y_{mn}(-x) = (-1)^{n-m} y_{mn}(x) \tag{6}$$

and similarly for H_{mn}.

The boundary conditions on equation (4) require that y be regular at $x = \pm 1$, i.e. near the endpoints the solution takes the form

$$y = c_0 + c_1(1 - x^2) + c_2(1 - x^2)^2 + \ldots . \tag{7}$$

On substituting this expansion into equation (4) and letting $x \to 1$, we obtain

$$c_1 = -\frac{\mu - c^2}{4(m+1)} c_0 \tag{8}$$

and so

$$y^1(1) = \frac{\mu - c^2}{2(m+1)} y(1). \tag{9}$$

A similar equation holds at $x = -1$ with a minus sign on the right-hand side. The irregular solution has a different relation between function and derivative at the endpoints.

Instead of integrating the equation from -1 to $+1$, we can exploit the symmetry (6) to integrate from 0 to 1. The boundary condition at $x = 0$ is

$$\begin{aligned} y(0) &= 0 \qquad && n - m \text{ odd} \\ y^1(0) &= 0 \qquad && n - m \text{ even.} \end{aligned} \tag{10}$$

A third boundary condition comes from the fact that any constant multiple of a solution y is a solution. This means that we can normalise the solution. We adopt the normalisation that the function H_{mn} has the same limiting behaviour as P_n^m at $x=1$, namely

$$\lim_{x\to 1}(1-x^2)^{-m/2}H_{mn}(x;\,c)=\lim_{x\to 1}(1-x^2)^{-m/2}P_n^m(x). \tag{11}$$

Various normalisation conventions in the literature are tabulated by Flammer (1957).

The imposition of these boundary conditions for the second-order equation (4) makes it an eigenvalue problem for λ or equivalently for μ. We write it in the standard form by setting

$$y_1=y \tag{12}$$

$$y_2=y^1 \tag{13}$$

$$y_3=\mu. \tag{14}$$

Then

$$y_1^1=y_2 \tag{15}$$

$$y_2^1=\frac{1}{1-x^2}[2x(m+1)y_2-(y_3-c^2x^2)y_1] \tag{16}$$

$$y_3^1=0. \tag{17}$$

In this notation the boundary condition at $x=0$ is

$$\begin{aligned} y_1&=0 \qquad n-m \text{ odd}\\ y_2&=0 \qquad n-m \text{ even.}\end{aligned} \tag{18}$$

At $x=1$ we have two conditions:

$$y_2=\frac{y_3-c^2}{2(m+1)}y_1 \tag{19}$$

$$y_1=\lim_{x\to 1}(1-x^2)^{-m/2}P_n^m(x)=\frac{(-1)^m(n+m)!}{2^m m!(n-m)!}\equiv\gamma. \tag{20}$$

The decision has now to be made on what numerical method to use. If we simply require a few isolated values of λ or H, shooting is probably the quickest method. Shooting methods (see Keller 1976) vary in their choice of initial or final conditions and in the integration of the equations in one direction or two directions. Newton's technique is the most widely known of the shooting methods and can be applied successfully to boundary-value problems of this type as long as the resulting initial-value problem is stable and a set of good guesses can be made for the unspecified conditions (see Kubicek and Hlavacek 1983). An up-to-date discussion of methods of this type is given by Constantinides (1987). However, the relaxation approach is preferable if we require values for a large sequence of values of c. Relaxation has the advantage that it rewards a good initial guess with rapid convergence. Also the previous solution should be a good initial guess if c is changed only slightly. A comparison of various collocation methods and finite-difference methods, including relaxation, for boundary-value problems of this type is given by Russell (1977).

2. Relaxation method

In relaxation methods we essentially replace ODE by approximate finite-difference equations on a grid or mesh of points which spans the domain of interest. To illustrate, we could replace a general first-order differential equation

$$y^1 = f(x, y) \tag{21}$$

with an algebraic equation relating function values at two points k, $k-1$ by using

$$y_k - y_{k-1} - (x_k - x_{k-1}) f(\tfrac{1}{2}(x_k + x_{k-1}), \tfrac{1}{2}(y_k + y_{k-1})) = 0. \tag{22}$$

Extending this to a system of N first-order ODE leads to an approximation by algebraic relations of the form

$$0 = \boldsymbol{R}_k = \boldsymbol{y}_k - \boldsymbol{y}_{k-1} - (x_k - x_{k-1}) \boldsymbol{f}_k(x_k, x_{k-1}, \boldsymbol{y}_k, \boldsymbol{y}_{k-1}) \qquad k = 2, 3, \ldots, M \tag{23}$$

using a mesh of M points.

The solution of the finite-difference equations (23) consists of a set of variables $y_{j,k}$, i.e. the values of the N variables y_j at the M points x_k. By taking an initial approximation for the $y_{j,k}$ it is possible to determine increments $\Delta y_{j,k}$ such that $y_{j,k} + \Delta y_{j,k}$ is an improved approximation to the solution.

First-order Taylor series with respect to small changes $\Delta \boldsymbol{y}_k$ are used to obtain equations for the increments. This gives at an interior point ($k = 2, 3, \ldots, M$)

$$\boldsymbol{R}_k(\boldsymbol{y}_k + \Delta \boldsymbol{y}_k, \boldsymbol{y}_{k-1} + \Delta \boldsymbol{y}_{k-1}) \simeq \boldsymbol{R}_k(\boldsymbol{y}_k, \boldsymbol{y}_{k-1}) + \sum_{n=1}^{N} \frac{\partial \boldsymbol{R}_k}{\partial y_{n,k-1}} \Delta y_{n,k-1} + \sum_{n=1}^{N} \frac{\partial \boldsymbol{R}_k}{\partial y_{n,k}} \Delta y_{n,k}. \tag{24}$$

For a solution the updated value of $\boldsymbol{R}(\boldsymbol{y} + \Delta \boldsymbol{y})$ should be zero and this leads to the general set of equations

$$\sum_{n=1}^{N} V_{j,n} \Delta y_{n,k-1} + \sum_{n=N+1}^{2N} V_{j,n} \Delta y_{n-N,k} = -R_{j,k} \qquad j = 1, 2, \ldots, N \tag{25}$$

where

$$V_{j,n} = \frac{\partial R_{j,k}}{\partial y_{n,k-1}} \qquad V_{j,n+N} = \frac{\partial R_{j,k}}{\partial y_{n,k}} \qquad n = 1, 2, \ldots, N. \tag{26}$$

The quantity $V_{j,n}$ is an $N \times 2N$ matrix at each point k. Thus each interior point supplies a block of N equations coupling $2N$ corrections to the solution variables at the points k, $k-1$.

In a similar way, the algebraic equations at the boundaries can be expanded in a first-order Taylor series for increments that improve the solution. Hence we have a set of linear equations to be solved for the corrections Δy, iterating until the corrections are sufficiently small. These equations have a special structure because each $V_{j,n}$ couples only points k, $k-1$.

3. Numerical solution by relaxation

In our case, for simplicity, we choose a uniform grid on the interval $0 \leqslant x \leqslant 1$. For a total of M mesh points, we have

$$h = 1/(m-1) \tag{27}$$

$$x_k = (k-1)h \qquad k = 1, 2, \ldots, M. \tag{28}$$

At interior points $k=2,3,\ldots,M$, equation (15) gives

$$R_{1,k}=y_{1,k}-y_{1,k-1}-\tfrac{1}{2}h(y_{2,k}+y_{2,k-1}). \tag{29}$$

Equation (16) gives

$$R_{2,k}=y_{2,k}-y_{2,k-1}-a_k[\tfrac{1}{2}(x_k+x_{k-1})(m+1)(y_{2,k}+y_{2,k-1})-\tfrac{1}{2}b_k(y_{1,k}+y_{1,k-1})] \tag{30}$$

where

$$a_k=h/[1-\tfrac{1}{4}(x_k+x_{k-1})^2] \tag{31}$$

$$b_k=\tfrac{1}{2}(y_{3,k}+y_{3,k-1})-\tfrac{1}{4}c^2(x_k+x_{k-1})^2. \tag{32}$$

Finally, equation (17) gives

$$R_{3,k}=y_{3,k}-y_{3,k-1}. \tag{33}$$

The matrix of partial derivatives $V_{i,j}$ of equation (26) is defined so that i labels the equation and j the variable. In our case, j runs from 1 to 3 for y_j at $k-1$ and from 4 to 6 for y_j at k. Thus equation (29) gives

$$\begin{aligned} &V_{1,1}=-1 \qquad V_{1,2}=-h/2 \qquad V_{1,3}=0\\ &V_{1,4}=1 \qquad V_{1,5}=-h/2 \qquad V_{1,6}=0. \end{aligned} \tag{34}$$

Similarly, equation (31) gives

$$\begin{aligned} &V_{2,1}=a_kb_k/2 \qquad V_{2,2}=-1-a_k(x_k+x_{k-1})(m+1)/2\\ &V_{2,3}=a_k(y_{1,k}+y_{1,k-1})/4 \qquad V_{2,4}=V_{2,1}\\ &V_{2,5}=2+V_{2,2} \qquad V_{2,6}=V_{2,3} \end{aligned} \tag{35}$$

while from equation (33) we have

$$\begin{aligned} &V_{3,1}=0 \qquad V_{3,2}=0 \qquad V_{3,3}=-1\\ &V_{3,4}=0 \qquad V_{3,5}=0 \qquad V_{3,6}=1. \end{aligned} \tag{36}$$

At $x=0$ we have the boundary condition

$$V_{3,1}=\begin{cases} y_{1,1} & n-m \text{ odd}\\ y_{2,1} & n-m \text{ even.}\end{cases} \tag{37}$$

We adopt the convention in the relaxation solution that for one boundary condition at $k=1$ only $V_{3,j}$ can be non-zero. Also, j takes on the values 4-6 since the boundary condition involves only y_k, not y_{k-1}. This means that the only non-zero values of $V_{3,j}$ at $x=0$ are

$$\begin{aligned} &V_{3,4}=1 \qquad n-m \text{ odd}\\ &V_{3,5}=1 \qquad n-m \text{ even.}\end{aligned} \tag{38}$$

At $x=1$ we have

$$R_{1,M+1}=y_{2,M}-\frac{y_{3,M}-c^2}{2(m+1)}y_{1,M} \tag{39}$$

$$R_{2,M+1}=y_{1,M}-\gamma. \tag{40}$$

Thus

$$V_{1,4}=-\frac{y_{3,M}-c^2}{2(m+1)} \qquad V_{1,5}=1 \qquad V_{1,6}=\frac{y_{1,M}}{2(m+1)} \tag{41}$$

$$V_{2,4}=1 \qquad V_{2,5}=0 \qquad V_{2,6}=0. \tag{42}$$

We now need a computer program to implement the above algorithm and to test out by computing the eigenvalues $\lambda_{mn}(c)$ for selected values of m, n and c.

4. Computed results

A computer program has been written which implements the above algorithm. It computes eigenvalues of spheroidal harmonics $H_{mn}(x; c)$ for $m \geqslant 0$ and $n \geqslant m$. For simplicity we choose an equally spaced mesh of $M = 41$ points, i.e. $h = 0.025$. This should give good accuracy for the eigenvalues up to moderate values of $n - m$.

Within the program, the set of linear equations (25) is solved by Gaussian elimination for the corrections Δy, iterating until the corrections are sufficiently small. It is best to use a form of Gaussian elimination which exploits the special structure of the matrix to minimise the total number of operations and which minimises storage of matrix coefficients by packing the elements in a special blocked structure.

Since the boundary condition at $x = 0$ does not involve y_1 if $n - m$ is even, it will be necessary to interchange the columns for y_1 and y_2 to avoid a zero pivotal element in the matrix $[V_{ij}]$.

Resulting from the above method a computer program is quickly available which computes eigenvalues of spheroidal harmonies $H_{mn}(x; c)$ for $m \geqslant 0$ and $n \geqslant m$. Also the program is highly interactive and prompts for values of m and n. This relaxation is preferable to the other methods previously discussed for the computation of values of λ and H for a large sequence of values of c. The important advantage is that a good initial guess is rewarded by rapid convergence, i.e. only a few iterations are required. Also a good initial guess is provided by the previous solution if c is changed only slightly.

The program has been run and checked against values of $\lambda_{mn}(c)$ given in the tables at the back of Flammer (1957) or in table 21.1 of Abramowitz and Stegun (1968). Typically it converges in about three iterations. A few comparisons are given in table

Table 1. Selected computed values of λ.

m	n	c^2	Computed λ	Exact λ
1	1	1.0	2.195 55	2.195 55
		4.0	2.734 11	2.734 11
		16.0	4.399 61	4.399 59
2	2	0.1	6.014 27	6.014 27
		1.0	6.140 95	6.140 95
		4.0	6.542 53	6.542 50
2	5	1.0	30.437 2	30.436 1
		16.0	37.013 5	36.996 3
4	11	−1.0	131.554	131.560

1 to demonstrate the high accuracy which can be achieved with a minimum of computational effort for eigenvalues up to moderate values of $n-m$. For the range of results quoted the accuracy is well within 0.05%. The alternative of using the power series expansion for λ_{mn} given in the appendix would require awkward terms beyond those up to $k=4$ quoted in the appendix to achieve this level of accuracy.

This point is illustrated in table 2 by comparing values of λ_{mn} up to $k=4$ in the power series expansion (A1) with both the relaxation and exact values for the case $m=n=1$. The alternative of using the asymptotic expansion (A2) is limited and only applies to large values of c.

Table 2. Comparison of values of λ_{mn} up to $k=4$ in the power series expansion (A1) with both the relaxation and exact values for the case $m=n=1$.

m	n	c^2	Power series λ (up to $k=4$)	Computed λ (relaxation)	Exact λ
1	1	1.0	2.195 55	2.195 55	2.195 55
		4.0	2.734 95	2.734 11	2.734 11
		16.0	4.604 23	4.399 61	4.399 59

Appendix. Power series and asymptotic expansions for λ_{mn}

A1. Power series expansion

It has been shown (see Abramowitz and Stegun 1963) that the power series expansion for λ_{mn} is given by

$$\lambda_{mn}=\sum_{k=0}^{\infty} l_{2k}c^{2k} \tag{A1}$$

where

$$l_0=n(n+1) \qquad l_2=\tfrac{1}{2}\left(1-\frac{(2m-1)(2m+1)}{(2n-1)(2n+3)}\right)$$

$$l_4=\frac{-(n-m+1)(n-m+2)(n+m+1)(n+m+2)}{2(2n+1)(2n+3)^3(2n+5)}+\frac{(n-m-1)(n-m)(n+m-1)(n+m)}{2(2n-3)(2n-1)^3(2n+1)}$$

$$l_6=(4m^2-1)\left(\frac{(n-m+1)(n-m+2)(n+m+1)(n+m+2)}{(2n-1)(2n+1)(2n+3)^5(2n+5)(2n+7)}-\frac{(n-m-1)(n-m)(n+m-1)(n+m)}{(2n-5)(2n-3)(2n-1)^5(2n+1)(2n+3)}\right)$$

$$l_8=2(4m^2-1)^2A+\tfrac{1}{16}B+\tfrac{1}{8}C+\tfrac{1}{2}D$$

where

$$A=\frac{(n-m-1)(n-m)(n+m-1)(n+m)}{(2n-5)^2(2n-3)(2n-1)^7(2n+1)(2n+3)^2}$$

$$-\frac{(n-m+1)(n-m+2)(n+m+1)(n+m+2)}{(2n-1)^2(2n+1)(2n+3)^7(2n+5)(2n+7)^2}$$

$$B=\frac{(n-m-3)(n-m-2)(n-m-1)(n-m)(n+m-3)(n+m-2)(n+m-1)(n+m)}{(2n-7)(2n-5)^2(2n-3)^3(2n-1)^4(2n+1)}$$

$$-\frac{\begin{array}{r}(n-m+1)(n-m+2)(n-m+3)(n-m+4)\\ \times(n+m+1)(n+m+2)(n+m+3)(n+m+4)\end{array}}{(2n+1)(2n+3)^4(2n+5)^3(2n+7)^2(2n+9)}$$

$$C=\frac{(n-m+1)^2(n-m+2)^2(n+m+1)^2(n+m+2)^2}{(2n+1)^2(2n+3)^7(2n+5)^2}$$

$$-\frac{(n-m-1)^2(n-m)^2(n+m-1)^2(n+m)^2}{(2n-3)^2(2n-1)^7(2n+1)^2}$$

$$D=\frac{(n-m-1)(n-m)(n-m+1)(n-m+2)(n+m-1)(n+m)(n+m+1)(n+m+2)}{(2n-3)(2n-1)^4(2n+1)^2(2n+3)^4(2n+5)}.$$

A2. Asymptotic expansion

Again it has been shown (see Abramowitz and Stegun 1968) that the asymptotic expansion for λ_{mn} is given by

$$\begin{aligned}\lambda_{mn}(c)=cq+m^2-\tfrac{1}{8}(q^2+5)-\frac{q}{64c}(q^2+11-32m^2)\\ -\frac{1}{1024c^2}[5(q^4+26q^2+21)-384m^2(q^2+1)]\\ -\frac{1}{c^3}\left(\frac{1}{128^2}(33q^5+1594q^3+5621q)-\frac{m^2}{128}(37q^3+167q)+\frac{m^4}{8}q\right)\\ -\frac{1}{c^4}\left(\frac{1}{256^2}(63q^6+4940q^4+43\,327q^2+22\,470)\right.\\ \left.-\frac{m^2}{512}(115q^4+1310q^2+735)+\frac{3m^4}{8}(q^2+1)\right)\\ -\frac{1}{c^5}\left(\frac{1}{1024^2}(527q^7+61\,529q^5+1043\,961q^3+2241\,599q)-\frac{m^2}{32\times1024}\right.\\ \left.\times(5739q^5+127\,550q^3+298\,951q)+\frac{m^4}{512}(355q^3+1505q)-\frac{m^6q}{16}\right)+\mathrm{O}(c^{-6})\end{aligned} \quad \text{(A2)}$$

$q=2(n-m)+1.$

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