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The asymptotic iteration method for the angular spheroidal eigenvalues

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Abstract

The asymptotic iteration method is applied to calculate the angular spheroidal eigenvalues $\lambda_{\ell}^{m}(c)$. It is shown that this method asymptotically gives accurate results over the full range of parameter values, ℓ , m and c.

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1. Introduction

The solution of the spheroidal wave equation is a very old subject, but it is still an important theme in the existing literature. The importance of this equation arises in different topics of physics such as the study of light scattering in optics [1], the nuclear shell model [2], theoretical cosmological models [3] and atomic and molecular physics [4]. In all these topics, trying to be more faithful to the geometry, the related physical system is expressed in the spheroidal coordinate system, the natural coordinate system for describing a revolution ellipsoid. Using the method of separation of variables in this coordinates system, the full wave equation can be written as products of radial and angular spheroidal wave equations. The radial spheroidal wave equation is always associated with a specified potential in each particular case, but the angular spheroidal wave equation is general.

In recent decades, there has been a steady amount of ongoing work on the solution of the angular spheroidal wave equation. Slepian [5] and Streifer [6] derived uniform asymptotic expansions for the spheroidal functions and their eigenvalues, which were further developed by des Cloiseaux and Mehta [7] and Dunster [8]. Other asymptotic results based on WKB methods have been obtained by Sink and Eu [9] and Guimaräes [10].

On the other hand, several packages have been developed for the computation of the angular spheroidal eigenvalues $\lambda_{\ell}^{m}(c)$. Thompson [11], Li *et al* [12, 13], and Falloon *et al* [14] are some of the most recent ones. All these attempts to obtain the eigenvalues $\lambda_{\ell}^{m}(c)$ rely very heavily on power series expansions and complicated recurrence relations. Accurate results in these works are obtainable at the expense of extensive mathematical and numerical manipulations.

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Here, this work applies the asymptotic iteration method [15, 16] for the computation of the angular spheroidal eigenvalues $\lambda_{\ell}^{m}(c)$, which is very easy to implement, and the results are sufficiently accurate for practical purposes.

The asymptotic iteration method puts no constraints on the parameter values involved such as ℓ , *m* and *c*. It also handles $\lambda_{\ell}^{m}(c)$ with large ℓ which pose many numerical instabilities in some of the previously mentioned methods. Therefore, the main motivation of the present work is to overcome the shortcomings of those approaches, and to formulate an elegant algebraic approach to yield a fairly simple analytic formula which will rapidly give the eigenvalues with high accuracy. To the best of our knowledge, this is the first time the asymptotic iteration method has been used to obtain the exact eigenvalues of the angular spheroidal wave equation.

In this spirit, this paper is organized as follows. In section 2 the asymptotic iteration method for the angular spheroidal wave equation is outlined. The analytical expressions for the asymptotic iteration method are cast in such a way that allows the reader to use them without proceeding into their derivation. In section 3 we present our numerical results, and then we conclude and remark therein.

2. Formalism of the asymptotic iteration method for the angular spheroidal wave equation

The angular spheroidal wavefunctions $S_{\ell,m}(c; \eta)$ satisfy the following second-order differential equation on the interval $-1 \leq \eta \leq 1$:

$$\frac{\mathrm{d}}{\mathrm{d}\eta} \left[(1-\eta^2) \frac{\mathrm{d}}{\mathrm{d}\eta} S_{\ell,m} \right] + \left[\left(\lambda_{\ell}^m(c) \right)^2 - c^2 \eta^2 - \frac{m^2}{(1-\eta^2)} \right] S_{\ell,m} = 0, \tag{1}$$

where ℓ , in this paper, is a positive integer ($\ell = 0, 1, ...$), the integer *m* defined in the range $-\ell \leq m \leq \ell$ is the L_z angular momentum eigenvalue (in units of $\hbar = 1$), $\lambda_{\ell}^m(c)$ are the angular spheroidal eigenvalues that is to be determined by solving equation (1) and *c* is the 'oblateness' parameter. Despite the notation, c^2 can be positive or negative. For $c^2 > 0$ the functions are called 'prolate', while if $c^2 < 0$ they are called 'oblate'.

Equation (1) has singular points at $\eta = \pm 1$, and is to be solved subject to the boundary conditions that the solution be regular at $\eta = \pm 1$. Only for certain values of $\lambda_{\ell}^{m}(c)$, the eigenvalues, will this be possible.

If we consider first the spherical case, where c = 0, the function $S_{\ell,m}(c; \eta)$ reduces to the associated Legendre function, and $(\lambda_{\ell}^m(c))^2 = \ell(\ell + 1)$ are its eigenvalues. Here, the integer ℓ labels successive eigenvalues for fixed m. When $\ell = m$ we have the lowest eigenvalue, and the corresponding eigenfunction has no nodes in the interval $-1 \le \eta \le 1$. When $\ell = m + 1$ 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 $c^2 \ne 0$.

In order to apply the asymptotic iteration method, we have to investigate the behaviour of the solution near the singular points $\eta = \pm 1$. Substituting a power series expansion of the form

$$S_{\ell,m}(c;\eta) = (1 \pm \eta^2)^{\alpha} \sum_{k=0}^{\infty} a_k (1 \pm \eta^2)^k,$$
(2)

into equation (1), we find that the regular solution has $\alpha = m/2$. Without loss of generality, we can take $m \ge 0$ since $m \to -m$ is a symmetry of the equation. Therefore, we get an equation that is more tractable to the method if we factor out this behaviour.

Accordingly, we set

$$S_{\ell,m}(c;\eta) = (1-\eta^2)^{m/2} y_{\ell,m}(c;\eta),$$
(3)

then the new function $y_{\ell,m}(c; \eta)$ will satisfy a second-order homogeneous linear differential equation of the form

$$(1 - \eta^2) \frac{d^2 y_{\ell,m}(c;\eta)}{d\eta^2} - 2(m+1)\eta \frac{d y_{\ell,m}(c;\eta)}{d\eta} + (\varepsilon - c^2 \eta^2) y_{\ell,m}(c;\eta) = 0,$$
(4)

where

$$\varepsilon \equiv \left(\lambda_{\ell}^{m}(c)\right)^{2} - m(m+1). \tag{5}$$

Both equations (1) and (4) are invariant under the replacement $\eta \rightarrow -\eta$. Thus the functions $S_{\ell,m}(c;\eta)$ and $y_{\ell,m}(c;\eta)$ must also be invariant, except possibly for an overall scale factor.

The systematic procedure of the asymptotic iteration method begins by rewriting equation (4) in the following form

$$y_{\ell,m}''(c;\eta) = \lambda_0(\eta) y_{\ell,m}'(c;\eta) + s_0(\eta) y_{\ell,m}(c;\eta),$$
(6)

where

$$\lambda_0(\eta) = \frac{2(m+1)\eta}{(1-\eta^2)}$$
 and $s_0(\eta) = -\frac{\varepsilon - c^2 \eta^2}{(1-\eta^2)}.$ (7)

The primes of $y_{\ell,m}(c; \eta)$ in equation (6) denote derivatives with respect to η .

Now, in order to find a general solution to this equation we rely on the symmetric structure of the right-hand side of equation (6). Thus, if we differentiate equation (6) with respect to η , we obtain

$$y_{\ell,m}^{\prime\prime\prime}(c;\eta) = \lambda_1(\eta) y_{\ell,m}^{\prime}(c;\eta) + s_1(\eta) y_{\ell,m}(c;\eta),$$
(8)

where

$$\lambda_1(\eta) = \lambda'_0(\eta) + s_0(\eta) + \lambda_0^2(\eta)$$
 and $s_1(\eta) = s'_0(\eta) + s_0(\eta)\lambda_0(\eta)$.

Likewise, the calculations of the second derivative of equation (6) yield

$$y_{\ell,m}^{\prime\prime\prime\prime}(c;\eta) = \lambda_2(\eta) y_{\ell,m}^{\prime}(c;\eta) + s_2(\eta) y_{\ell,m}(c;\eta),$$
(9)

where

$$\lambda_2(\eta) = \lambda_1'(\eta) + s_1(\eta) + \lambda_0(\eta)\lambda_1(\eta) \quad \text{and} \quad s_2(\eta) = s_1'(\eta) + s_0(\eta)\lambda_1(\eta)$$

Thus, for (n + 1)th and (n + 2)th derivatives, n = 1, 2, ..., we have

$$y_{\ell,m}^{(n+1)}(c;\eta) = \lambda_{n-1}(\eta)y_{\ell,m}'(c;\eta) + s_{n-1}(\eta)y_{\ell,m}(c;\eta),$$
(10)

and

$$y_{\ell,m}^{(n+2)}(c;\eta) = \lambda_n(\eta) y_{\ell,m}'(c;\eta) + s_n(\eta) y_{\ell,m}(c;\eta),$$
(11)

respectively, where

$$\lambda_n(\eta) = \lambda'_{n-1}(\eta) + s_{n-1}(\eta) + \lambda_0(\eta)\lambda_{n-1}(\eta) \quad \text{and} \quad s_n(\eta) = s'_{n-1}(\eta) + s_0(\eta)\lambda_{n-1}(\eta).$$
(12)

The ratio of the (n + 2)th and (n + 1)th derivatives can be expressed as

$$\frac{\mathrm{d}}{\mathrm{d}\eta}\ln(y_{\ell,m}^{(n+1)}(c;\eta)) = \frac{y_{\ell,m}^{(n+2)}(c;\eta)}{y_{\ell,m}^{(n+1)}(c;\eta)} = \frac{\lambda_n(y_{\ell,m}'(c;\eta) + \frac{s_n}{\lambda_n}y_{\ell,m}(c;\eta))}{\lambda_{n-1}(y_{\ell,m}'(c;\eta) + \frac{s_{n-1}}{\lambda_{n-1}}y_{\ell,m}(c;\eta))}.$$
 (13)

For sufficiently large n, we can now introduce the 'asymptotic' aspect of the method, that is

$$\frac{s_n(\eta)}{\lambda_n(\eta)} = \frac{s_{n-1}(\eta)}{\lambda_{n-1}(\eta)} \equiv \beta(\eta), \tag{14}$$

thus equation (13) can be reduced to

$$\frac{\mathrm{d}}{\mathrm{d}\eta}\ln\left(\mathbf{y}_{\ell,m}^{(n+1)}(c;\eta)\right) = \frac{\lambda_n(\eta)}{\lambda_{n-1}(\eta)},\tag{15}$$

which yields

$$y_{\ell,m}^{(n+1)}(c;\eta) = C_1 \exp\left(\int \frac{\lambda_n(\eta)}{\lambda_{n-1}(\eta)} \,\mathrm{d}\eta\right) = C_1 \lambda_{n-1}(\eta) \exp\left(\int (\beta(\eta) + \lambda_0(\eta)) \,\mathrm{d}\eta\right),\tag{16}$$

where C_1 is the integration constant, and the right-hand of equation (16) follows from equation (12), and the definition of β . Substituting equation (16) into equation (10) we obtain a first-order differential equation

$$y'_{\ell,m}(c;\eta) + \beta(\eta)y_{\ell,m}(c;\eta) = C_1 \exp\left(\int (\beta(\eta) + \lambda_0(\eta)) \,\mathrm{d}\eta\right),\tag{17}$$

which, in turn, yields the general solution to equation (6)

$$y_{\ell,m}(c;\eta) = \exp\left(-\int^{\eta} \beta(\eta') \, \mathrm{d}\eta'\right) \left[C_2 + C_1 \int^{\eta} \exp\left(\int^{\eta'} \{\lambda_0(\eta'') + 2\beta(\eta'')\} \, \mathrm{d}\eta''\right) \, \mathrm{d}\eta'\right].$$
(18)

Perhaps it should be noted that one can construct the spheroidal wavefunctions $S_{\ell,m}(c; \eta)$ from knowledge of β . The work on this issue is in progress, and is planned to be reported briefly. However, such a study lies beyond the scope of our methodical proposal.

3. Numerical results for the angular spheroidal eigenvalues $\lambda_{\ell}^{m}(c)$

Within the framework of the asymptotic iteration method mentioned in section 2, the angular spheroidal eigenvalues $\lambda_{\ell}^{m}(c)$ are calculated by means of equation (14). To obtain the eigenvalues $\lambda_{\ell}^{m}(c)$ the iterations should be terminated by imposing a condition $\delta_{n}(\eta) = 0$ as an approximation to equation (14). On the other hand, for each iteration, the expression $\delta_{n}(\eta) = s_{n}(\eta)\lambda_{n-1}(\eta) - s_{n-1}(\eta)\lambda_{n}(\eta)$ depends on two variables: $\lambda_{\ell}^{m}(c)$ and η . The calculated eigenvalues $\lambda_{\ell}^{m}(c)$ by means of this condition should, however, be independent of the choice of η . Nevertheless, the choice of η is observed to be critical only to the speed of the convergence to the eigenvalues, as well as for the stability of the process. In this work it is observed that the best starting value for η is that value at which the effective potential of equation (1) takes its minimum value. For this purpose, it is necessary to perform the variable change $\eta \to \tanh(x)$, mapping the finite interval (-1, 1) into the infinite one $(-\infty, \infty)$, then equation (1) can be rewritten as

$$-\frac{d}{dx^2}S_{\ell,m} + V_{\text{eff}}(x)S_{\ell,m} = -m^2 S_{\ell,m},$$
(19)

where the effective potential $V_{\text{eff}}(x)$ is

$$V_{\rm eff}(x) = -\left[\left(\lambda_{\ell}^{m}(c)\right)^{2} - c^{2}\right]\operatorname{sech}^{2}(x) - c^{2}\operatorname{sech}^{4}(x).$$
(20)

 $V_{\text{eff}}(x)$ is an even function, its minimum value occurs when x = 0, which in turn implies that $\eta = 0$. Therefore, at the end of the iterations we put $\eta = 0$.

The results of the asymptotic iteration method for $\lambda_{\ell}^{m}(c)$ with different values of ℓ , *m* and *c* are reported in tables 1, 2, 3 and 4. In tables 1, 3 and 4 the angular spheroidal eigenvalues $\lambda_{\ell}^{m}(c)$ were calculated by means of 25 iterations only. While, in table 2, in order to reproduce more accurate results, the angular spheroidal eigenvalues $\lambda_{\ell}^{m}(c)$ were calculated by means of 33 iterations. The predicted eigenvalues $\lambda_{\ell}^{m}(c)$ are all in excellent agreement with the exact ones [9, 12, 17].

Table 1. A comparison between the exact eigenvalues $(\lambda_{\ell}^{m}(c))^{2}$ and the eigenvalues computed by means of this work with 25 iterations for c = 1 and m = 0.

$\left(\lambda_{\ell}^{m}(c) ight)^{2}$					
l	Exact [9]	Equation (14)			
0	0.3190	0.3190			
1	2.5931	2.5931			
2	6.5335	6.5335			
3	12.5145	12.5145			
4	20.5083	20.5083			
5	30.5054	30.5054			
6	42.5038	42.5038			
7	56.5028	56.5028			
8	72.5022	72.5022			
9	90.5017	90.5017			

Table 2. A comparison between the exact eigenvalues $(\lambda_{\ell}^{m}(c))^{2}$ and the eigenvalues computed by means of this work with 33 iterations for c = 8 and m = 0.

$\left(\lambda_{\ell}^{m}(c)\right)^{2}$					
l	Exact [9]	Equation (14)			
0	7.2216	7.2216			
1	22.0921	22.0921			
2	35.7064	35.7064			
3	47.7571	47.7571			
4	58.0167	58.0167			
5	67.3646	67.3647			
6	77.8251	77.8252			
7	90.6913	90.6914			
8	106.0116	106.0116			
9	123.5771	123.5771			

Table 3. A comparison between the exact eigenvalues $(\lambda_{\ell}^m(c))^2$ and the eigenvalues computed by means of this work with 25 iterations for c = 8 and $m = \ell$.

$ig(\lambda_\ell^m(c)ig)^2$						
l	т	Exact [9]	Equation (14)			
0	0	7.2216	7.2216			
1	1	8.3000	8.3000			
2	2	11.5278	11.5278			
3	3	16.8867	16.8867			
4	4	24.3549	24.3549			
5	5	33.9121	33.9121			
6	6	45.5411	45.5411			
7	7	59.2276	59.2276			
8	8	74.9605	74.9605			
9	9	92.7310	92.7310			

The results of this work have shown that the asymptotic iteration method is very easy to implement for calculating the angular spheroidal eigenvalues $\lambda_{\ell}^{m}(c)$, and it is quite flexible in the sense that it works very well over the full range of parameter values. Moreover, the obtained

$\left(\lambda_\ell^m(c)\right)^2$						
l	т	c^2	Exact [12]	Equation (14)		
2	2	0.1	6.01427	6.01427		
2	2	1	6.14095	6.14095		
2	2	4	6.54250	6.54250		
5	2	1	30.4361	30.4361		
5	2	16	36.9963	36.9963		
11	4	-1.0	131.560	131.560		

Table 4. Selected output of eigenvalues $(\lambda_{\ell}^{m}(c))^{2}$ computed by means of this work with 25 iterations for different values of c, ℓ and m.

eigenvalues are not limited by the magnitude of c, and satisfy a simple ordering relation. Therefore, we can unambiguously select the correct starting eigenvalue. This represents a significant advantage over the tridiagonal matrix method [14] in which the eigenvalues are not in order, and hence to choose the correct matrix eigenvalue, one must use an iterative process to move towards the starting value.

As a concluding remark, we would like to point out that the accuracy of the results increases as the number of iterations increases, and this method can be applied to compute the eigenvalues with arbitrary complex parameters.

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