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SPHEROIDAL WAVE FUNCTIONS

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SPHEROIDAL WAVE FUNCTIONS OCCUR IN MANY SCIENTIFIC AND ENGINEERING CONTEXTS, FROM ATOMIC NUCLEI TO THE COSMOS—SCATTERING BY NONSPHERICAL NUCLEI, WAVE FUNCTIONS OF DIATOMIC MOLECULES, ANALYSIS OF BAND-LIMITED random noise, orthogonal frequency division multiplexing, and anisotropy of the cosmic microwave background radiation. Therefore, visualizing these functions and computing them reliably can be useful and interesting.

What are spheroidal wave functions?

Spheroidal wave functions are generalizations of Legendre functions and spherical Bessel functions for spheroidal coordinates rather than for the spherical polar coordinates in which the latter functions usually occur. The literature on spheroidal wave functions is often in the context of specialized applications, but two applied-mathematics monographs are especially useful: those by Julius Stratton and colleagues[1] and by Carson Flammer.[2] Josef Meixner and colleagues have derived analytical results,[3,4] and summaries of many results appear in *Higher Transcendental Functions*, edited by Arthur Erdélyi,[5] and in the *Handbook of Mathematical Functions*, edited by Milton Abramowitz and Irene Stegun.[6] For extensive discussions of computational methods—with programs in Mathematica, C, and Fortran—see my atlas of mathematical functions.[7]

Spheroidal coordinates

I relate spheroidal coordinates—d, h, x, and f—to Cartesian coordinates—x, y, and z—as in Flammer's monograph:[2] For *prolate* coordinates,

$$x = \frac{d}{2}\sqrt{\left(1-\eta^2\right)\left(\xi^2-1\right)}\cos\phi$$
$$y = \frac{d}{2}\sqrt{\left(1-\eta^2\right)\left(\xi^2-1\right)}\sin\phi\,,$$

$z = d\eta\xi/2$, $-1 \le \eta \le 1$, $\xi \ge 1$, and $0 \le \phi \le 2\pi$. For *oblate* coordinates,

$$x = \frac{d}{2}\sqrt{\left(1-\eta^2\right)\left(\xi^2+1\right)}\cos\phi$$
$$y = \frac{d}{2}\sqrt{\left(1-\eta^2\right)\left(\xi^2+1\right)}\sin\phi\,,$$

$z = d\eta\xi/2$, $-1 \le \eta \le 1$, $\xi \ge 0$, and $0 \le \phi \le 2\pi$.

The limits $\xi \to \infty$, $d \to 0$, $d\xi/2 = r$, and $\eta = \cos\theta$ produce spherical polar coordinates. Many of the spheroidal coordinate systems used by other authors, including Abramowitz and Stegun, do not have this limit property. Figure 1 illustrates surfaces corresponding to constant parameter values—η, ξ, or ϕ. The parameter d provides an overall scale factor, as does r in spherical polar coordinates. For details of the geometry of spheroidal coordinates, see the references by Flammer,[2] Abramowitz and Stegun,[6] and Parry Moon and Domina Spencer.[8] Beware, the choice of coordinate systems and notations is quite variable!

The scalar wave equation in spheroidal coordinates

As a context for spheroidal wave functions, consider solving the scalar wave equation in spheroidal coordinates. The related, but more complicated, vector wave equation for Maxwell's equations is covered by Flammer, by Moon and Spencer, and in technical papers on antenna theory and wave scattering by spheroids.

The scalar wave equation for wave number k—namely, $\nabla^2\psi + k^2\psi = 0$—is separable in spheroidal coordinates by writing, for prolate coordinates,

$$\psi_{mn} = S_{mn}(c,\eta)R_{mn}(c,\xi)\left|\begin{matrix}\cos m\phi\\ \sin m\phi\end{matrix}\right.,$$

in which m is an integer if the ϕ dependence has a period of 2π and if n is an integer. This separability is analogous to that for solving the Laplace equation ($k = 0$) in spherical polar coordinates. Function S_{mn} is the *prolate spheroidal angular function* when k is real, because in the limit of small nonsphericity, η becomes the polar angle θ. Parameter c is given by $c \equiv kd/2 = \pi d/\lambda$, where λ is the wavelength corresponding to wave number k. Thus, c scales as the ratio of distance to wavelength. Function R_{mn} is the *prolate spheroidal radial function*, which becomes a spherical Bessel function in the limit of zero c.

Prolate spheroidal functions satisfy Equation 1 for the angular function and Equation 2 for the radial function. (See the sidebar for all numbered equations.) In these equations, $\lambda_{mn}(c)$ is the *prolate spheroidal eigenvalue*, with $\lambda_{mn}(0) = n(n + 1)$. Oblate coordinates have a similar separation of the wave equation.

Equations

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

$$\frac{d}{d\xi}\left[\left(\xi^2-1\right)\frac{dR_{mn}(c,\xi)}{d\xi}\right]-\left[\lambda_{mn}-c^2\xi^2+\frac{m^2}{\xi^2-1}\right]R_{mn}(c,\xi)=0 \qquad (2)$$

$$\gamma_r^m \equiv (m+r)(m+r+1)+\frac{c^2}{2}\left[1-\frac{4m^2-1}{(2m+2r-1)(2m+2r+3)}\right] \qquad (3)$$

$$\beta_r^m \equiv \frac{r(r-1)(2m+r)(2m+r-1)c^4}{(2m+2r-1)^2(2m+2r-3)(2m+2r+1)} \qquad (4)$$

$$U_1(\lambda_{mn}) \equiv \gamma_{n-m}^m-\lambda_{mn}-\cfrac{\beta_{n-m}^m}{\gamma_{n-m-2}^m-\lambda_{mn}-\cfrac{\beta_{n-m-2}^m}{\gamma_{n-m-4}^m-\lambda_{mn}-\ldots}} \qquad (5)$$

$$U_2(\lambda_{mn}) \equiv -\cfrac{\beta_{n-m+2}^m}{\gamma_{n-m+2}^m-\lambda_{mn}-\cfrac{\beta_{n-m+4}^m}{\gamma_{n-m+4}^m-\lambda_{mn}-\ldots}} \qquad (6)$$

$$R_{mn}^{(1)}(c,\xi)=\left(1-1/\xi^2\right)^{m/2}\sum_{r=0,1}^{\infty}a_r^{mn}(c)\,j_{m+r}(c\xi) \qquad (7)$$

Analytical results for spheroidal wave functions are commonly presented in terms of those for prolate functions. The transition to the oblate functions (angular or radial functions, or eigenvalues) follows this rule: prolate ↔ oblate by $c \leftrightarrow \pm ic$, $c^2 \leftrightarrow -c^2$. However, all spheroidal functions are real-valued, in spite of this rule's appearance. In the following, I give results for prolate functions, with the understanding that the rule is used in analysis (but not in numerical computations!) to obtain results for oblate functions. In a dispersive (lossy) medium, the wave number k is a complex number, so c is complex. Le-Wei Li and his colleagues have considered this case.[9]

Spheroidal wave functions are usually expanded in a basis of corresponding spherical functions, with the magnitude of c controlling the range of basis functions needed for accurate results.

Eigenvalues for spheroidal equations

The eigenvalues, λ_{mn}, are tricky, tedious, and time-consuming to compute accurately. I present the necessary formulas; for their derivation, see Flammer's monograph.[2] Here I describe a brute-force method.

First, we define two functions that depend on m, n, and c (but not on the eigenvalue), shown in Equations 3 and 4. Then, we combine these functions to define two functions of λ_{mn}, shown in Equations 5 and 6. The first continued fraction terminates with either the term containing γ_0^m or the term with γ_1^m, depending on whether $n - m$ is even or odd, while the second fraction is nonterminating (in principle). As the second fraction's upper limit increases, the accuracy with which λ_{mn} can be determined increases.

The eigenvalue λ_{mn} is the root of the transcendental equation $U(\lambda_{mn}) \equiv U_1(\lambda_{mn}) + U_2(\lambda_{mn}) = 0$. This equation has no closed-form solutions, except if $c = 0$ when $\lambda_{mn} = n(n + 1)$ or if the deformation is large. Accurate eigenvalues are the essential first step for determining spheroidal wave functions. Approximate eigenvalues can be estimated by expanding them as power series in c or as asymptotic series in c and its inverse powers. The resulting cumbersome formulas are accurate to better than parts per million only for very small or very large c. If the interfocal distance of the spheroidal coordinates $d \approx \lambda$, a condition that is often interesting, then $c \approx 3$. For such c values, the series formulas give an accuracy of only a few percent for most values of m and n.

For m and n from 0 to 6, and for c with a magnitude less than 3, the eigenvalues have a uniform, slow dependence on deformation parameter c. For oblate and prolate cases, $\lambda_{mn}(c)$ deviates from the spherical coordinates value, $n(n + 1)$, in opposite directions. This deviation is consistent with the leading term in a power series expansion in c being quadratic. When the magnitude of c is small, the effects of nonsphericity generally become smaller as n increases.

To compute the eigenvalues numerically, we can start with approximate solutions derived from power series or asymptotic expansions, then refine these solutions by a robust root-finding algorithm. Using either starting method gives

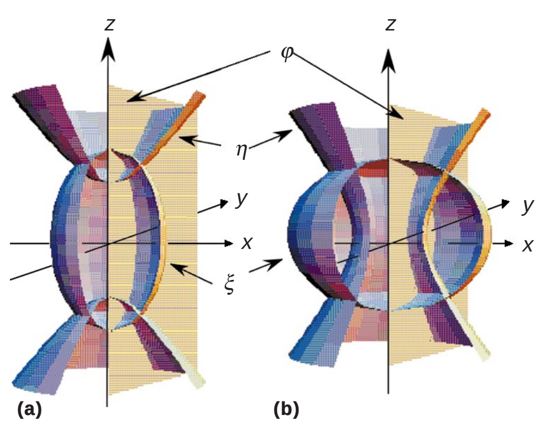

Figure 1. Spheroidal coordinates: (a) prolate; (b) oblate. η, ξ, and ϕ are constant parameter values. Coordinate surfaces are hyperboloids of revolution for η, and half planes for ϕ.

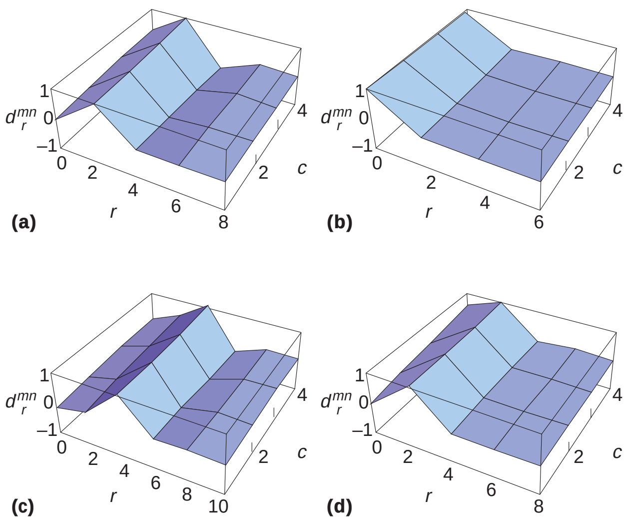

Figure 2. Coefficients for expanding spheroidal wave functions in a basis of Legendre functions, for *m* and *n* values of (a) 0, 2; (b) 2, 2; (c) 0, 4; and (d) 2, 4. The coefficients peak at *r* = *n* – *m*, which is the unique value when the prolateness parameter *c* = 0.

eigenvalue estimates that are usually within 0.2 of the final eigenvalue. We can therefore use a simple and robust root finder, such as the bisectional method, to locate the roots. Typically, a dozen bisections produce part-per-thousand accuracy in $\lambda_{mn}(c)$, and approximately 30 bisections results in 10-digit accuracy, the goal for functions in my atlas.[7]

When c is small in magnitude, the eigenvalue departs steadily from the spherical-coordinates value. You might therefore expect that the eigenvalue equation's roots are unique, as some previous investigations have assumed. However, as m and n increase, this is not necessarily so.[3,4,7]

Spheroidal angular functions

Spheroidal angular functions are usually expanded into spherical Legendre functions of the first kind, $\mathrm{P}_{m+r}^{m}(\eta)$, or the second kind, $\mathrm{Q}_{m+r}^{m}(\eta)$.

For functions of the first kind, which are regular at $\eta = \pm 1$, we write

$$S_{mn}^{(1)}(c,\eta) = \sum_{r=0,1}^{\infty} d_r^{mn}(c)\mathrm{P}_{m+r}^{m}(\eta) ,$$

with summation starting at $r = 0$ if $n - m$ is even but at $r = 1$ if $n - m$ is odd. In either case, r goes by steps of two. As $c \to 0$, the spheroidal angular function collapses to $\mathrm{P}_{m+r}^{m}(\eta)$ with the same m and n values. The only nonzero angular coefficient is then $d_{n-m}^{mn}(c)$, corresponding to $r = n - m$. For functions of the second kind, which are irregular at $\eta = \pm 1$, we have

$$S_{mn}^{(2)}(c,\eta) = \sum_{r=0,1}^{\infty} d_r^{mn}(c)\mathrm{Q}_{m+r}^{m}(\eta) .$$

As $c \to 0$, this collapses to $Q_n^m(\eta)$, so that the only nonzero angular coefficient is $d_{n-m}^{mn}(c)$—that is, $r = n - m$.

We can compute spheroidal angular coefficients $d_r^{mn}(c)$ from the recurrence relation

$$\alpha_r d_{r+2}^{mn} + \left(\beta_r - \lambda_{mn}\right) d_r^{mn} + \gamma_r d_{r-2}^{mn} = 0,$$

with α_r and γ_r given by

$$\alpha_r = \frac{(2m+r+2)(2m+r+1)c^2}{(2m+2r+3)(2m+2r+5)}$$

and

$$\gamma_r = \frac{r(r-1)c^2}{(2m+2r-3)(2m+2r-1)} .$$

Recurrence can procede in the direction of increasing or decreasing r. For modest values of $n - m$, the latter gives more accurate results.

(Computing has certainly progressed over the last 40 years. The 75,000 numerical values that Stratton and colleagues used required "about six months of fairly intensive effort" from two programmers and 10 hours of production time on MIT's Whirlwind I computer.[1] The output was more than five kilometers of paper tape, from which they prepared tables on an electric typewriter. A modern desktop computer reduces both the execution time and the computer's volume by factors of approximately 1,000.)

Expansion coefficients for the angular part of spheroidal wave functions depend on the order n, the degree m, and the parameter c, and on whether you are using prolate or oblate coordinates. Figure 2 displays the $d_r^{mn}(c)$ values as surfaces made from plaquettes whose vertices are the coefficient values. The coefficients for oblate coordinates behave similarly to those for prolate coordinates. If c^2 is much larger than shown here, however, the behavior of the $d_r^{mn}(c)$ becomes complicated.

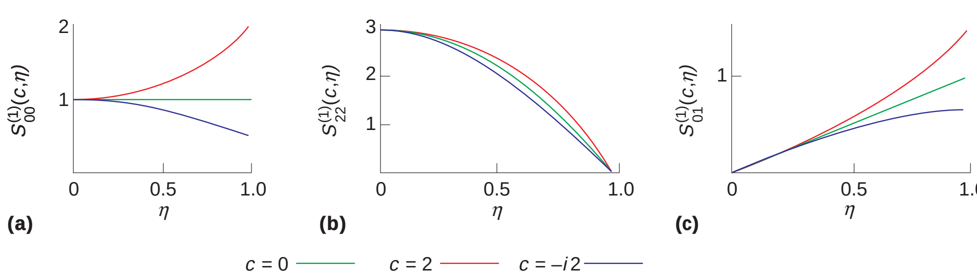

Figure 3. Spheroidal angular functions of the first kind, for prolate (*c* = 2), spherical (*c* = 0), and oblate (*c* = –*i*2) coordinates, for *m* and *n* values of (a) 0, 0; (b) 2, 2; and (c) 0, 1.

There are four arguments for each spheroidal angular function of the first and second kind: m, n, c, and η. To visualize $S^{(1)}_{mn}(c,\eta)$, we choose $|c| = 2$ and superimpose three curves for each m and n: $c = 2$ (prolate case), $c = 0$ (spherical case), and $|c| = 2$ (oblate case). For $c = 0$, we have the spherical Legendre functions, $P^m_n(\eta)$. For the regular functions, Figure 3 shows $S^{(1)}_{mn}(c,\eta)$ for η over [0, 1]. The spherical angular function is nearly the average of the values for prolate and oblate coordinates, indicating that the $d^{mn}_r(c)$ are approximately even functions of c.

Spheroidal radial functions

The spheroidal radial functions, $R_{mn}(c, \xi)$, are usually expanded in a basis of spherical Bessel functions.[7] The expansions are quite simple, because radial expansion coefficients are proportional to angular expansion coefficients. A given set of spherical-basis radial functions (Bessel, Neumann, or Hankel) has corresponding spheroidal radial functions. I discuss the spheroidal radial function called $R^{(1)}_{mn}(c, \xi)$ by Flammer,[2] by Abramowitz and Stegun,[6] and in my atlas,[7] but called $je_{m\ell}(b, \xi)$ by Stratton and colleagues,[1] where $\ell = n$ and $b = c$ in our notation. When $c = 0$, $R^{(1)}_{mn}(c, \xi)$ collapses to $j_n(c\xi)$, the spherical Bessel function.

The prototype spheroidal radial function is regular at $\xi = \pm 1$ and expands in terms of regular spherical Bessel functions as shown in Equation 7. In this equation, summation starts at $r = 0$ if $n - m$ is even but at $r = 1$ if $n - m$ is odd. In either case, r goes by steps of two. The coefficients $a^{mn}_r(c)$ are *radial expansion coefficients*. As $c \to 0$, the spheroidal radial function collapses to $j_n(c\xi)$, and the only nonzero radial coefficient is then $a^{mn}_{n-m}(0)$, corresponding to $r = n - m$.

We can readily compute the spheroidal radial coefficients in terms of the angular coefficients d^{mn}_r. Although the normalization of the angular coefficients is different between Stratton and colleagues[1] and Flammer,[2] the radial coefficients are the same. Figure 4 displays the $a^{mn}_r(c)$ values as surfaces made from plaquettes whose vertices are the radial coefficient values. To visualize $R^{(1)}_{mn}(c, \xi)$, I choose $|c| = 2$ and show two curves for each m and n: $|c| = 2$ (prolate coordinates) and $c = -i2$ (oblate coordinates), as in Figure 5.

After we have computed the angular and radial spheroidal wave functions, we can compute the complete spheroidal wave function, which can help solve many problems of interest to scientists and engineers.

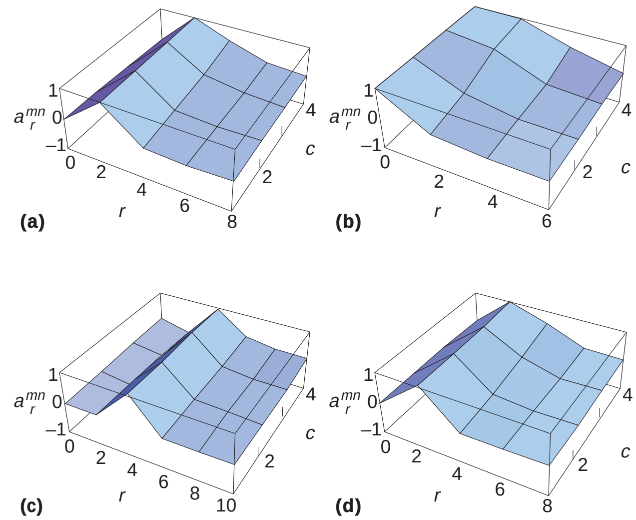

Figure 4. Radical coefficients for expansion into spherical Bessel functions, for *m* and *n* values of (a) 0, 2; (b) 2, 2; (c) 0, 4; and (d) 2, 4. The coefficients peak at *r* = *n* – *m*, the unique value when *c* = 0.

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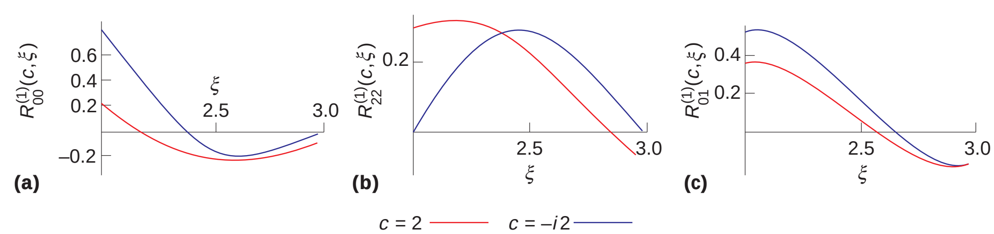

Figure 5. Spheroidal radial functions of the first kind for prolate (*c* = 2) and oblate (*c* = –*i*2) coordinates for *m* and *n* values of (a) 0, 0; (b) 2, 2; and (c) 0, 1.