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INTRODUCTION

The morphology dependent resonances are of growing interest due to their extremely high quality factor. The quality factor, or Q factor, is a dimensionless parameter that indicates the energy loss relative to the stored energy within a resonant element. The higher the Q, the lower the rate of energy loss and as a result the slower the oscillations will die out. An overview about the current state of research on the MDR can be found in [1].

The numerical simulation of these phenomena is not straightforward, even in the case of symmetry allowing the separation of variables in the modeling equations. Below, we report on a progress made in the numerical simulation of the so called 'whispering gallery' modes occurring inside a prolate spheroid. The approach presented here is also applicable for any other separable geometry.

PROLATE SPHEROIDAL COORDINATES AND PROLATE SPHEROIDAL WAVE FUNCTIONS

Here, we collect the most important facts, concerning the problem setting, for more details see [2] and the literature therein.

Prolate spheroidal coordinates are introduced via their relation to the conventional Cartesian coordinates,

$$x = \frac{d}{2}\sqrt{(\xi^2-1)(1-\eta^2)}\cos\varphi, \quad y = \frac{d}{2}\sqrt{(\xi^2-1)(1-\eta^2)}\sin\varphi, \quad z = \frac{d}{2}\xi\eta,$$

where $\varphi \in [0, 2\pi)$ is the azimuthal angle, while $\eta \in (-1,1)$ and $\xi \in (1,\infty)$ play the roles of inclination and radius, respectively. The corresponding coordinate surfaces are confocal two-sheeted hyperboloids of revolution and prolate spheroids with d being the distance between the foci.

As $\xi \to \infty$, the prolate spheroidal coordinates transform asymptotically to spherical coordinates $\xi = 2r/d$, $\eta = \cos\theta$.
The eigenvalue problem for the Laplace operator defined on the domain bounded by a spheroid $\xi = \xi_0$,

$$-\Delta W(\mathbf{r}) = k^2 W(\mathbf{r}), \quad \mathbf{r} = (\varphi, \eta, \xi), \quad \xi < \xi_0,$$

is separable in spheroidal coordinates, provided that either Dirichlet or Neumann boundary conditions are imposed. Any particular solution of the problem is now represented as a product of its angular, radial, and azimuthal component,

$$W(\mathbf{r}) = S(\eta)R(\xi)\exp(\pm im\varphi), \quad m = 0,1,\ldots,$$

where $S(\eta)$ and $R(\xi)$ are bounded solutions of the angular and radial prolate spheroidal wave equations, respectively,

$$\frac{d}{d\eta}(1-\eta^2)\frac{d}{d\eta}S + \left[\lambda + c^2(1-\eta^2) - \frac{m^2}{1-\eta^2}\right]S = 0, \quad -1 < \eta < 1 \tag{1}$$

and

$$\frac{d}{d\xi}(\xi^2 - 1)\frac{d}{d\xi}R + \left[c^2(\xi^2 - 1) - \lambda - \frac{m^2}{\xi^2 - 1}\right]R = 0, \quad 1 < \xi < \xi_0. \tag{2}$$

In (1) and (2), $c = kd/2$, with k being the dimensionless wave number. Note that the differential operators in (1) and (2) exhibit two singular points at $\eta = \pm 1$, and one singular point at $\xi = 1$, respectively. Due to the symmetry of the problem, angular functions S are either odd or even, and therefore, one can consider (1) on the half-interval $[0, 1)$, imposing either condition $S(0) = 0$ or $S'(0) = 0$. The boundary condition for the eigenfunction $W(\mathbf{r})$ implies either $R(\xi_0) = 0$ or $R'(\xi_0) = 0$. In addition, both $S(\eta)$ and $R(\xi)$ are normalized by

$$\int\limits_{-1}^{1} S^2(\eta)\,d\eta = 1, \quad \int\limits_{1}^{\xi_0} R^2(\xi)\,d\xi = 1.$$

BOUNDARY CONDITIONS TRANSFER TO A REGULAR POINT

Let us fix indexes $l, n, m \in \mathbb{N}$. The numerical technique presented below is not applicable to singular differential equations, therefore we shall formulate an equivalent problem on the domain $(0, 1 - \delta_\eta) \times (1 + \delta_\xi, \xi_0)$ with $\delta_\eta > 0$ and $\delta_\xi > 0$ chosen to exclude singular points from the integration interval.

Let us first consider problem (1). Here, the singularity at the point $\eta = 1$ is indeed regular [3]. Unless $m = 0$, equation (1) has two linearly independent solutions $S^{(1)}(\eta) \sim (1 - \eta^2)^{m/2}$ and $S^{(2)}(\eta) \sim (1 - \eta^2)^{-m/2}$. The case $m = 0$ is characterized by the different asymptotical behavior of the solution near the singularities. In this case problem (1) has two linearly independent solutions $S^{(1)}(\eta) \sim \text{const}$ and $S^{(2)}(\eta) \sim \ln(1 - \eta^2), \ \eta \to 1$. In any case only $S^{(1)}$ is bounded.

For equation (2), the singularity at the point $\xi = 1$ is again regular. This means that for any solution bounded at $\xi = 1$ and $\xi \to 1$

$$R(\xi) \sim \begin{cases} \text{const} & \text{for } m = 0, \\ (\xi^2 - 1)^{m/2} & \text{for } m = 1, 2, \ldots \end{cases}$$

holds.

All solutions of (1) bounded at $\eta = 1$ have the same (modified) logarithmic derivative $\beta(\eta)$ defined by

$$(1 - \eta^2)\frac{d}{d\eta}S(\eta) = \beta(\eta)S(\eta). \tag{3}$$

Note that the logarithmic derivative β of any solution to (1) satisfies the Riccati equation,

$$\beta'(\eta) + \frac{\beta^2(\eta)}{1 - \eta^2} + Q(\eta) = 0. \tag{4}$$

However, the function β corresponding to the bounded solution of (1), additionally satisfies $\lim_{\eta \to 1 - 0} \beta(\eta) = -m$. In the vicinity of $\eta = 1$, there exists a unique solution to (4), which can be represented in form of an absolutely and uniformly convergent series $\beta(\eta) = \sum_{k=0}^{\infty} \beta_k (1 - \eta)^k$, with known coefficients [4], where $\beta_0 = -m$. Although the cases $m = 0$ and $m \neq 0$ have to be considered separately, the final formulas are consistent. Thus equation (3) transfers the boundedness condition from the singular point $\eta = 1$ to a closely located regular point.

Similarly, the boundedness condition for the radial solution part is transferred to a regular point ξ,

$$(\xi^2 - 1)\frac{d}{d\xi}R(\xi) = \tilde{\beta}(\xi)R(\xi), \quad \tilde{\beta}(\xi) = \sum_{k=0}^{\infty} \tilde{\beta}_k (\xi - 1)^k. \tag{5}$$

NUMERICAL TECHNIQUE

Although the independent variables in (1) and (2) are different, both equations remain linked through the separation constant λ as well as the unknown eigenfrequency c and hence, they form a two-parameter self-adjoint spectral problem.

The general theory for two- and multi-parameter spectral problems is now well-developed; for a comprehensive review see [5, 6]. It is known that for a given arbitrary pair of indexes $l, n \in \mathbb{R}$, functions $S_{ln}(\eta)$ and $R_{ln}(\xi)$ exist that satisfy (1) and (2) and oscillate l and n times within their definition intervals, respectively. Besides, function families S_{ln} and R_{ln} consist of pairwise orthogonal functions forming an orthonormal bases in $\mathscr{L}^2(0,1)$ and $\mathscr{L}^2(1,\xi_0)$.

However since the above problem is multiparameter and singular, its numerical solution even in the simplest cases requires special care. In [10] a numerical technique was proposed for evaluation of the angular ellipsoidal (Lamé) wave functions. This technique is universal and, with minor changes, can be applied to a wide class of two- and multi-parameter spectral problems [7, 8, 9].

The key role in the calculations plays the so called Prüfer angle – an auxiliary function that is introduced to single out the subspace of solutions satisfying one of the boundary conditions. We use a modification of the conventional Prüfer angle, which is free from the well-known drawback – the stepwise behavior – yet keeping on the possibility to count the number of zeros that the related solutions have between the interval endpoint and the current argument value. We emphasize that in calculations based on the Prüfer angle approach, the eigenvalues and eigenfunctions are computed for an *a priory* chosen multi-index, i.e. a tuple of integers defining the numbers of oscillations of separated angular and radial components.

WHISPERING GALLERY MODE AND SIMILAR HIGHLY LOCALIZED OSCILLATIONS

The Prüfer angle technique is based on the WKB[1] asymptotics of an oscillating solution of a second order ODE. The higher the number of oscillations, the larger the benefit of the method. However, if the real physical oscillations are concentrated within a narrow sub-domain bounded by caustics, only one of the separated eigenfunction components oscillates rapidly, while two others practically do not oscillate. This means that for the 'whispering gallery modes', as well as for other extremely high localized modes the Prüfer angle technique [7, 8, 9, 10] cannot be successfully applied. The reason is, that the direct calculations of the Prüfer angle of non-oscillating components becomes unstable and does allow neither to detect the eigenvalue nor to recover these components. In spite of the unstable behavior, it still can be used to localize the eigenvalue and provide a very accurate initial guess for the Newton iterations.

In the recent paper [11], we have combined the Prüfer angle method and the high order difference schemes for the evaluation of the hyper-spheroidal functions. The difference schemes enable calculations in cases that could not be performed using the Prüfer angle technique (see examples in Figures 4 to 6 [11]). Note that the power expansions do not help in these cases either.

Summarizing, for the scalar wave equation, we developed an efficient and reliable numerical technique for investigation of a wide spectrum of 'internal boundary value problems' arising inside resonator cavities of special geometries.

FINITE DIFFERENCE SCHEMES FOR THE HYPER-SPHEROIDAL FUNCTION

As in [12, 13], we discretize the equations (1) and (2) on equidistant meshes with n_1 and n_2 points and the stepsizes h_1 and h_2, respectively. Due to the singularities in the points $\eta = 1$ and $\xi = 1$, the first equation is discretized on $[0, 1-\delta_\eta]$, while the second one on $[1+\delta_\xi, \xi_0]$. Boundary conditions for the new end points, $1-\delta_\eta$ and $1+\delta_\xi$ are computed using (3), (4), and (5).

The finite difference schemes have the form

$$y_i^{(\nu)} = \frac{1}{h^\nu} \sum_{j=-s}^{r} \alpha_{j+s}^{(\nu)} y_{i+j}, \qquad \nu = 1, 2,$$

where h is the stepsize, $\alpha_i^{(\nu)}$ are the coefficients chosen in such a way that the formula has maximal consistency order, and $y_i \approx S(\eta_i)$ for $i = 1, \ldots, n_1$ or $y_i \approx R(\xi_i)$ for $i = 1, \ldots, n_2$. In the inner grid points we approximate the equations by means of central difference formulae ($r = s$) while, in the points located in the boundary regions, we use different stencils [12, 13].
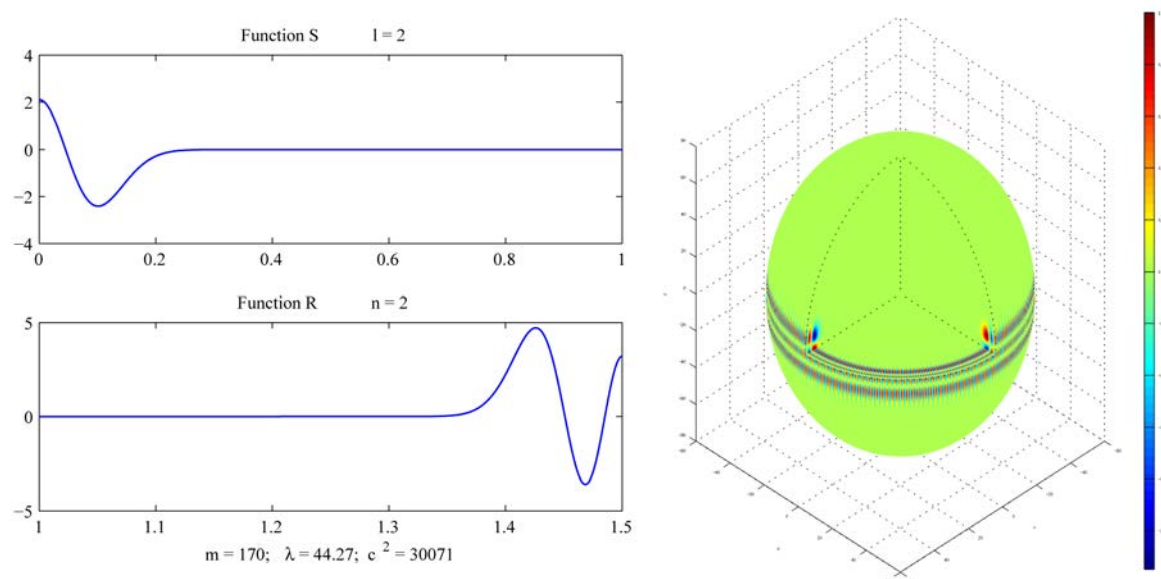
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[1] The Wentzel-Kramers-Brillouin (WKB) method is a procedure often applied to solve linear partial differential equations with coefficients depending on the space variable. It is often used in quantum mechanics, where the wave function is recast in the form of an exponential function.

The discrete problem

$$((I - D_\eta^2)A - 2D_\eta B + \lambda I + c^2(I - D_\eta^2) - m^2(I - D_\eta^2)^{-1})S = 0,$$
$$((D_\xi^2 - I)A + 2D_\xi B + c^2(D_\xi^2 - I) - \lambda I - m^2(D_\xi^2 - I)^{-1})R = 0, \tag{6}$$
$$h_1 S^T D_1 S = 0, \quad h_2 R^T D_2 R = 0,$$

consists of a nonlinear system with $n_1 + n_2 + 2$ equations, obtained from the discretization of equations (1) and (2) and from the normalization conditions. The $n_1 + n_2 + 2$ unknowns are $S(\eta_i)$, $i = 1, \ldots, n_1$, and $R(\xi_i)$, $i = 1, \ldots, n_2$, and the eigenvalues λ, c^2. In (6), vectors S and R contain the discrete values for $S(\eta_i)$ and $R(\xi_i)$ and the diagonal matrices D_x contain the values x_i for $x = \eta, \xi$. Matrices D_1 and D_2 are derived from the quadrature formulae approximating the normalization conditions and matrices A and B contain the coefficients of the methods.

The system is solved by the Newton iteration which works well if a good initial guess for the solution of (6) is provided. Therefore, we utilize λ and c^2 from the Prüfer angle procedure and decouple system (6) into two systems with $n_1 + 1$ and $n_2 + 1$ equations to calculate the initial approximations for the discrete eigenvector functions.

FIGURE 1. Whispering gallery mode: $m = 170$, $l = n = 2$, $\xi_0 = 1.5$, $S'(0) = 0$, $R'(\xi_0) = 0$.

The numerical solution shown in Figure 1 was obtained using the finite difference scheme of order 6 with $n_1 = n_2 = 1600$ and $\delta_\eta = \delta_\xi = 1e - 5$. The maximum norm of the estimated global error is around $1e - 7$.

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